National Aeronautics and
Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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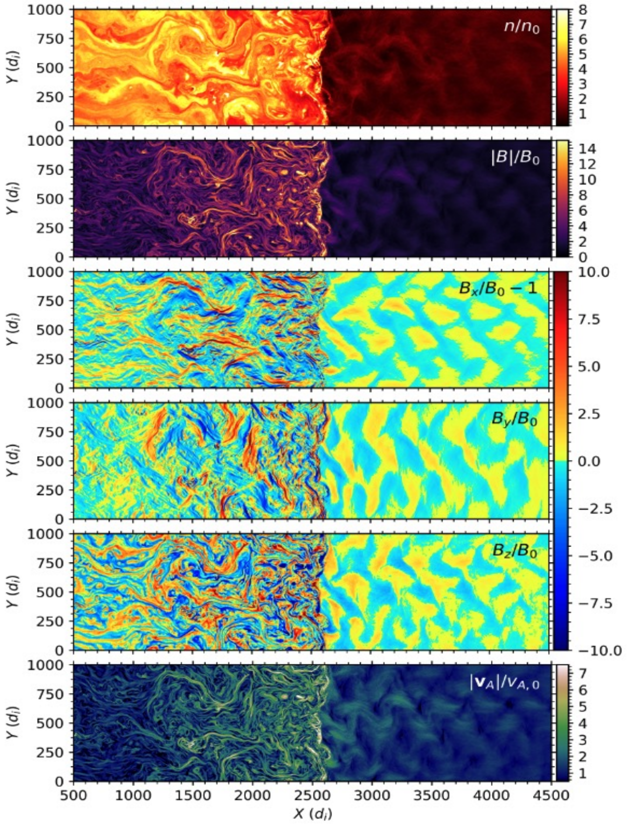
November 10, 2021

APP Team Makes Significant Improvements to Performance of Astrophysics Code

- HECC's Application Performance and Productivity (APP) team improved the performance of the dHybridR code by 5.6 times.
  - ***dHybridR*** is the first hybrid-PIC (particle in cell) simulation software to include relativistic proton dynamics and is ideal for studying the *ab initio* generation and transport of cosmic rays, which account for the highest energy particles in the universe.
  - An outstanding problem in Cosmic Ray (CR) acceleration is the backreaction of CRs on the shockwaves from supernova remnants. The computational cost has limited the range of shock velocities (or Mach numbers) that can be simulated using the hybrid model, with the largest Mach numbers only reaching about 80, as opposed to real supernovae with Mach numbers reaching 1,000.
- To improve dHybridR's performance, the APP team used a variety of tools to locate performance bottlenecks and then addressed the issues causing each bottleneck. Specifically, the team:
  - Rearranged the memory layout of key arrays.
  - Restructured the code to allow the compiler to vectorize important loops.
- In addition, the APP team searched dHybridR for latent bugs. That investigation led the team to find and fix an issue that resulted in a runtime failure.

IMPACT: The HECC optimizations applied to *dHybridR,* along with increasing supercomputer capabilities, will allow NASA to explore an important and previously inaccessible parameter regime.

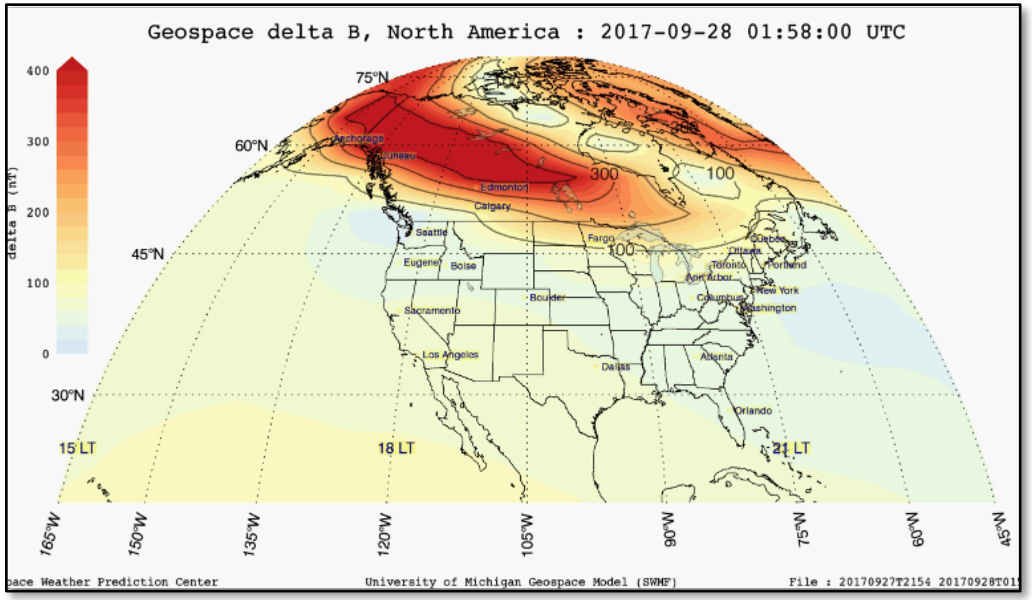


This image shows *dHybridR* simulation quantities from the shock wave in a Supernova Remnant. Quantities plotted from top to bottom: number density; magnetic field magnitude; x, y and z components; and local Alfvén speed—all normalized to the upstream value. *Colby Haggerty, University of Hawaii*

APP Team Speeds Up Space Weather Code by 13%

- HECC's Application Performance and Productivity (APP) team recently improved the performance of the Space Weather Modeling Framework (SWMF) code by 13%.
  - Space weather incorporates the various processes in the Sun–Earth system that present dangers to human health and technology.
- The goal of space weather forecasting is to provide an opportunity to mitigate negative effects such as:
  - Disturbances in satellite communication/navigation systems and radio communications.
  - Disruptions of power grids and systems, especially in the high-latitude areas.
  - Radiation effects on humans, which can be significant for astronauts and are non-negligible for crew and passengers on commercial aircraft.
- The APP team used a variety of tools to locate performance bottlenecks and then addressed the issues causing each bottleneck. Specifically, the team:
  - Restructured code in ten locations to allow the compiler to generate more efficient executable code.
  - Used the knowledge gained from code review and performance reports to determine a set of compiler flags that further improved performance.

IMPACT: The HECC team's optimizations applied to SWMF improves time to solution of the operational model and allows more science to be done on a given computational resource.

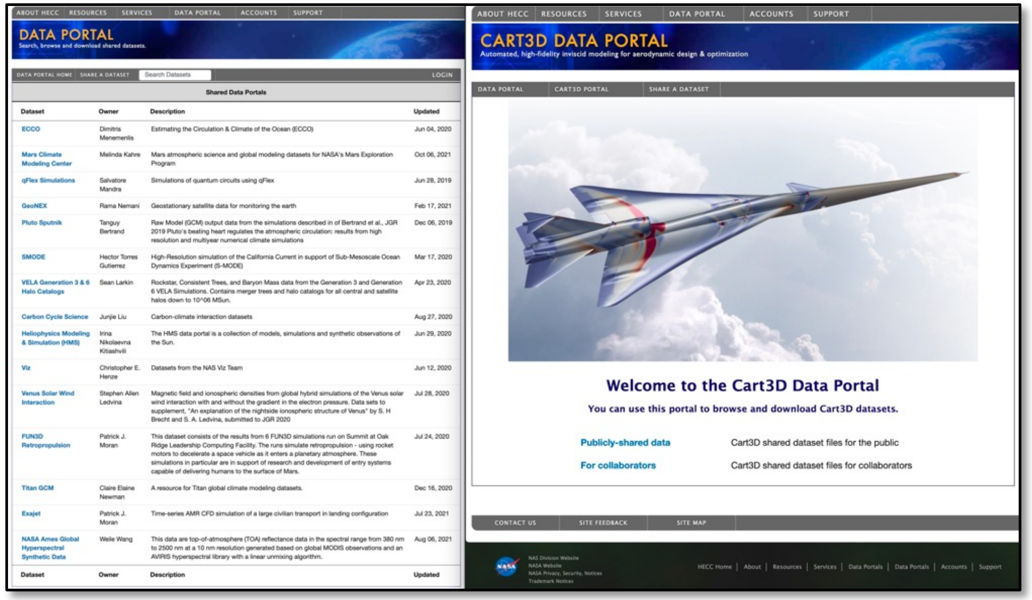


Prediction of local magnetic disturbances by the SWMF Geospace model. *Gabor Toth, University of Michigan*

New Data Portal Features Improve Usability

- In order to better serve the expanding data portal user base, several key features were added to the NAS Data Portal.
- Downloading dataset files in bulk can now be done more easily using a custom implementation of the “wget” command.
  - This command enables recursive downloads of all files and subdirectories, using concise command syntax.
  - This feature addresses a popular user request, as shared datasets grow to millions of files.
- Dataset owners can now publish changes themselves by running a custom “force” command on their dataset.
  - “Force” automates the sharing of dataset files and directories without affecting the source data directories on the /nobackup filesystem.
  - The command is accessible to all members of the owner’s NAS group, and available via a provided custom binary file on request.
- The “Private dataset” feature enables sharing with specific collaborators, which can now include non-NASA affiliates.
- A future upgrade enables local server storage to be used to continue serving critical files when the source dataset filesystems are unreachable.

IMPACT: New Data Portal features make it easier to share datasets for both dataset owners and recipients. As this capability evolves, new enhancements continue to be driven by requests from our user base.



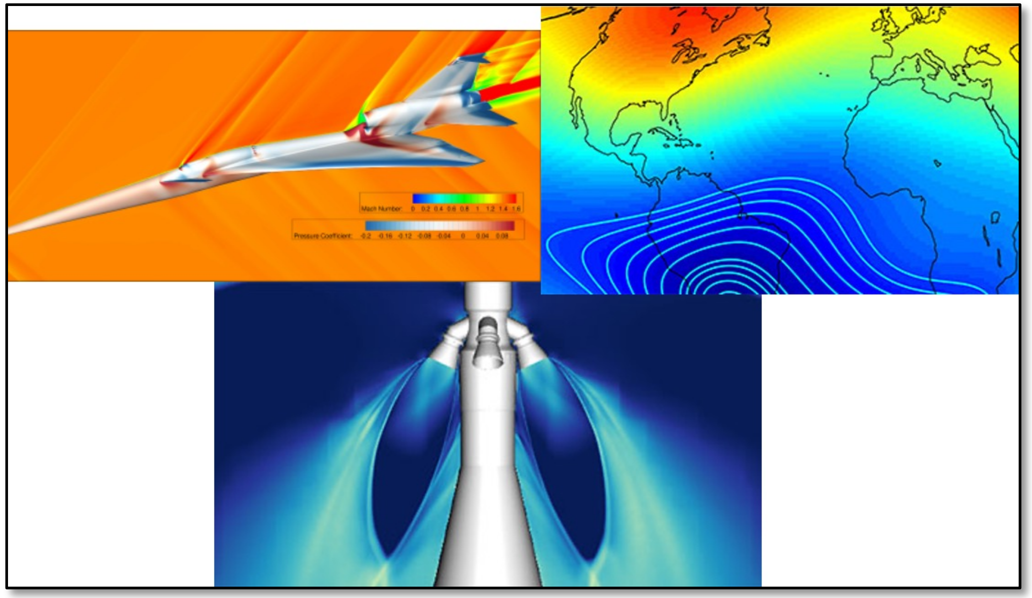
Left: The NAS Data Portal splash page allows access to the individual dataset portals. Right: The Cart3D database portal contains links to publicly available Cart3D data and (for designated collaborators) private Cart3D data. *Glenn Deardorff, NASA/Ames*

New Operational Period for Supercomputer Time Begins for NASA Mission Directorates

- The new allocation period for all NASA mission directorates began October 1.
  - Mission directorates were allocated approximately 183.5 million Standard Billing Units (SBUs)* to 630 projects.
  - The Aeronautics Mission Directorate allocated just under 51 million SBUs to 142 projects.
  - The Human and Operations Mission Directorate, Space Technology Mission Directorate, and NASA Engineering and Safety Center Mission Directorate collectively allocated more than 39 million SBUs to 62 projects.
  - The Science Mission Directorate allocated more than 93 million SBUs to 426 projects.
- This allocation period marked the first year that all mission directorates used the Request Management System (RMS) for requesting and allocating time (see slide 7).
  - The transition to the new system was smooth.
  - All principal investigator requests for changes to allocations will now be tracked in a single location.

** 1 SBU equals 1 hour of a Broadwell 28-core node*

IMPACT: NASA programs and projects periodically review the distribution of supercomputer time to assess demand for resources and assure consistency with mission-specific goals and objectives.



Clockwise from left: Flow visualization for a sample computational fluid dynamics solution of the X-59 aircraft concept; predicted geomagnetic field intensity at the Earth's mean surface in 2025; snapshot from a simulation of launch ignition for NASA's next-generation Space Launch System.

Successful NOP on Request Management System (RMS)

- HECC, in collaboration with NCCS, replaced REI eBooks with RMS in March 2021 for all mission directorates. This is the third New Operational Period (NOP) for SMD using the RMS, but the first NOP for the other mission directorates using https://request.hec.nasa.gov.
- An RMS information session for users, held on June 28, 2021, covered how to use the new system and Q&A.
- The NOP process went smoothly, with fewer issues than in prior years with eBooks and dispositions of allocation were made faster.
- The RMS tool enables new features such as:
  - Easy to navigate requests from the home screen: request more resources, request more time, cancel requests, or print PDFs.
  - Enables bulk allocation through Excel, rather than doing each allocation by hand.
  - Greater flexibility in customization and significant cost savings.
- Since July 2021 we have released nine enhancement versions, utilizing Agile methods that allow for continuous improvement.
- Upcoming major features include the ability to transition to HECC from the Goddard Private Cloud and being able to request commercial cloud resources through the RMS request form.

IMPACT: Developing in-house software to manage supercomputer resource allocation requests allows NASA's High End Computing Program more ownership of the data and simplifies the process for reviewing allocations and targets.

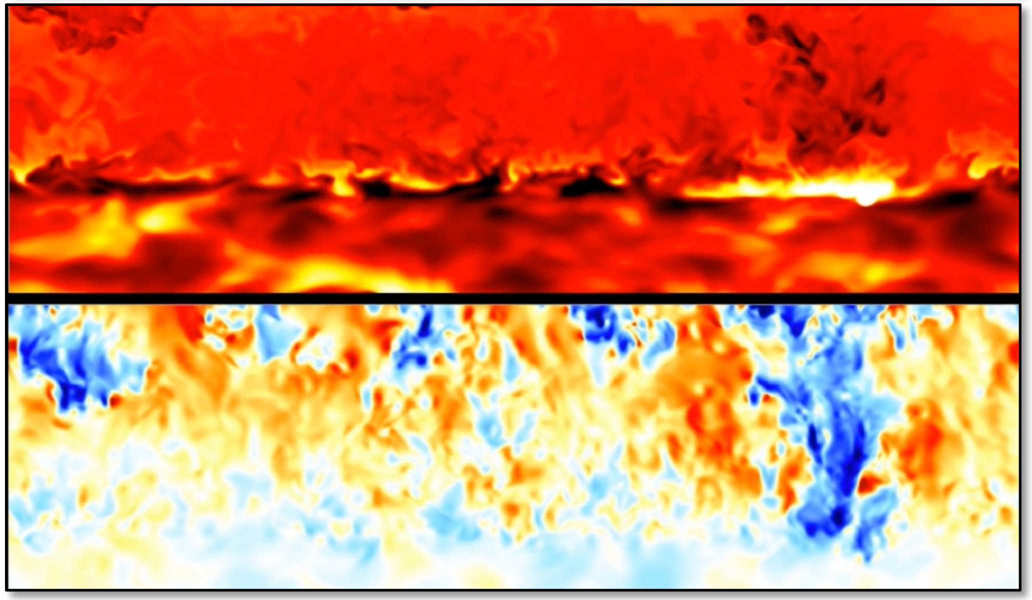
Slide from a High-End Computing Board of Advisors presentation for the Resource Management System. *NASA*

3D Realistic Modeling of Rotating Stars

- To support the dramatic increase in observational data from Kepler, K2, and TESS missions and from ground-based observatories, researchers at NASA Ames are building 3D dynamical and radiation models of stars from physical first principles.
- The team modeled a star of 1.47 solar mass (an F-type star) with a relatively shallow convection zone of 30,000 km, as compared with the Sun's 200,000-km convection zone, in order to:
  - Investigate the star's turbulent dynamics from the radiative zone to the outer convection zone and the surface, and at different latitudes.
  - Gain understanding of the origin of differential rotation, the excitation of stellar oscillation modes, and the dynamics and structure of the stellar tachocline.
- Simulation results revealed that:
  - The stellar surface is covered by multi-scale convective structures (granules) that are much larger than solar granules.
  - The equatorial regions of an F-type star, rotating within a one-day period, rotate more slowly than the star's polar regions. This behavior is opposite that of the Sun, where the equatorial regions rotate faster than the polar regions in its 27-day average period.
- These results improve the understanding of the internal dynamics, structures, and rotation periods of stars—critical for interpreting observational data.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: These models open opportunities for validating existing data analysis techniques and for interpreting observational data in terms of the physical processes inside stars.

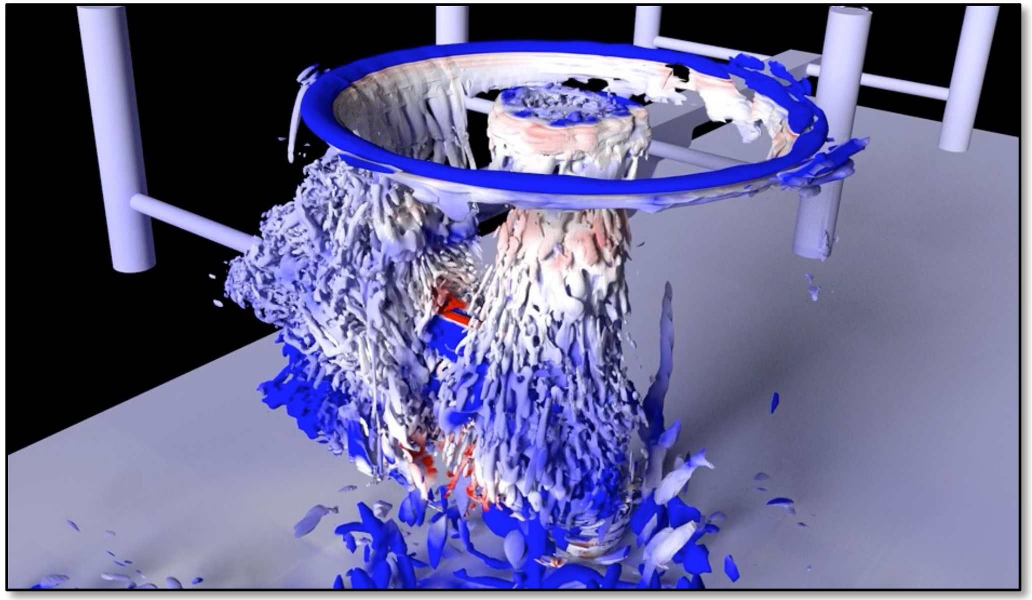


Video showing the internal dynamics beneath the surface of a star. At top: Temperature fluctuations, where darker colors correspond to lower temperatures and brighter colors to higher temperatures. At bottom: The radial velocity of stellar convection, where blue colors represent downflows and red upflows. *Irina Kitiashvili, Alan Wray, NASA/Ames*

Simulating Complex Multirotor Test Bed Systems

- Researchers at NASA Ames ran computational fluid dynamics (CFD) simulations of the agency's Multirotor Test Bed (MTB) system on HECC systems to capture rotor blade aerodynamics, blade and rotor performance, and rotor-body interactions.
  - Developed as part of NASA's Revolutionary Vertical Lift Technology Project, the MTB facilitates wind-tunnel testing for new and existing multirotor aircraft configurations, with a focus on collecting data for unmanned aircraft system (UAS) vehicles.
  - The MTB is designed to allow researchers and engineers to adjust the vertical, lateral, and longitudinal placement of each rotor, as well as the rotor tilt and the pitch of the whole aircraft assembly.
  - Wind tunnel geometry was included in the CFD model, allowing rotor-rotor interactions and interactions with the other components of the tunnel to be simulated, to ensure parity with experimental data.
  - To reduce the complexity of simulating unsteady flows of the rotating blades with moving overset grids, the team used an option in NASA's OVERFLOW code to model rotors and propellers as infinitely thin disks following disk actuator theory. Both full rotor and disk models were coupled with comprehensive rotorcraft analysis software and tested on various rotor systems.
- CFD methods developed by researchers in the NASA Advanced Supercomputing Division at Ames will be used as design and simulation tools for the next generation of rotor-based UAS and other concept vehicles. The rotor disk model used for the MTB will be utilized to accelerate the process.

IMPACT: High-fidelity CFD simulations run on HECC systems are necessary for representing the complex flow physics of multirotor vehicles in detail, helping NASA improve understanding and performance of multirotor systems.



Video of the modeled Multirotor Test Bed system in hover, showing flows inside the wind tunnel. The simulation shows the vortical structure mapped with the coefficient of pressure. *Jasim Ahmad, Tim Sandstrom, NASA/Ames*

Papers

- "**Introducing the THESAN Project: Radiation-Magneto-Hydrodynamic Simulations of the Epoch of Reionization**," R. Kannan, et al., arXiv:2110.00584 [astro-ph.GA], October 1, 2021. *
  https://arxiv.org/abs/2110.00584
- "**Self-Consistent Ring Model in Protoplanetary Disks: Temperature Dips and Substructure Formation**," S. Zhang, et al., arXiv:2110.00858 [astro-ph.EP], October 2, 2021. *
  https://arxiv.org/abs/2110.00858
- "**Derivation of Bedrock Topography Measurement Requirements for the Reduction of Uncertainty in Ice Sheet Model Projections of Thwaites Glacier**," B. Castleman, et al., The Cryosphere (Preprint), October 5, 2021. *
  https://tc.copernicus.org/preprints/tc-2021-274/
- "**Investigation of Species-Mass Diffusion in Binary-Species Boundary Layers at High Pressure Using Direct Numerical Simulation**," T. Toki, J. Bellan, Journal of Fluid Dynamics, vol. 928, October 6, 2021. *
  https://www.cambridge.org/core/journals/journal-of-fluid-mechanics/article/abs/investigation-of-speciesmass-diffusion-in-binaryspecies-boundary-layers-at-high-pressure-using-direct-numerical-simulations/CB097F58C20A766E1BC4DBD587E9672C
- "**Numerical Simulations of Convective 3-Dimensional Red Supergiant Envelopes**," J. Goldberg, Y.-F. Jiang, L. Bildsten, arXiv:2110.03261 [astro-ph.SR], October 7, 2021. *
  https://arxiv.org/abs/2110.03261

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**TOI-530b: A Giant Planet Transiting an M Dwarf Detected by TESS**," T. Gan, et al., arXiv:2110.04220 [astro-ph.EP], October 8, 2021. *
  https://arxiv.org/abs/2110.04220
- "**Turning AGN Bubbles into Radio Relics with Sloshing: Modeling CR Transport with Realistic Physics**," J. ZuHone, et al., arXiv:2110.04443 [astro-ph.HE], October 9, 2021. *
  https://arxiv.org/abs/2110.04443
- "**The TESS-Keck Survey. VI. Two Eccentric Sub-Neptunes Orbiting HIP-97166**," M. MacDougall, et al., arXiv:2110.05628 [astro-ph.EP], October 11, 2021. *
  https://arxiv.org/abs/2110.05628
- "**Streaming Instability with Multiple Dust Species – II. Turbulence and Dust-Gas Dynamics at Non-Linear Saturation**," C.-C. Yang, Z. Zhu, Monthly Notices of the Royal Astronomical Society, vol. 508, issue 4, October 14, 2021. *
  https://academic.oup.com/mnras/article-abstract/508/4/5538/6396762
- "**Boundary Layers of Accretion Disks: Discovery of Vortex-Driven Modes and Other Waves**," M. Coleman, et al., Monthly Notices of the Royal Astronomical Society, October 14, 2021. *
  https://academic.oup.com/mnras/advance-article-abstract/doi/10.1093/mnras/stab2962/6396757

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- “**HD207897 b: A Dense Sub-Neptune Transiting a Nearby and Bright K-type Star**,” N. Heidari, et al., arXiv:2110.08597 [astro-ph.EP], October 16, 2021. *
https://arxiv.org/abs/2110.08597
- “**TESS Hunt for Young and Maturing Exoplanets (THYME) VI: An 11 Myr Giant Planet Transiting a Very Low-Mass Star in Lower Centaurus**,” A. Mann, et al., arXiv:2110.09531 [astro-ph.EP], October 18, 2021. *
https://arxiv.org/abs/2110.09531
- “**TOI-2285b: A 1.7 Earth-radius Planet Near the Habitable Zone around a Nearby M Dwarf**,” A. Fukui, et al., arXiv:2110.10215 [astro-ph.EP], October 19, 2021. *
https://arxiv.org/abs/2110.10215
- “**Stellar Convective Penetration: Parameterized Theory and Dynamical Simulations**,” E. Anders, et al., arXiv:2110.11356 [astro-ph.SR], October 21, 2021. *
https://arxiv.org/abs/2110.11356
- “**Jet Launching from Merging Magnetized Binary Neutron Stars with Realistic Equations of State**,” M. Ruiz, et al., arXiv:2110.11968 [astro-ph.HE], October 22, 2021. *
https://arxiv.org/abs/2110.11968

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Papers (cont.)

- "**Entropy-Stable Schemes in the Low-Mach-Number Regime: Flux-Preconditioning, Entropy Breakdowns, and Entropy Transfers**," A. Gouasmi, et al., arXiv:2110.11941 [physics.flu-dyn], October 22, 2021. *
https://arxiv.org/abs/2110.11941
- "**The Young HD 73583 (TOI-560) Planetary System: Two 10-$M_\oplus$ Mini-Neptunes Transiting a 750-Myr-old, Bright, and Active K Dwarf**," O. Barragan, et al., arXiv:2110.13069 [astro-ph.EP], October 25, 2021. *
https://arxiv.org/abs/2110.13069
- "**TESS-Keck Survey. V. Twin Sub-Neptunes Transiting the Nearby G Star HD 63935**," N. Scarsdale, et al., The Astronomical Journal, vol. 162, no. 5, October 26, 2021. *
https://iopscience.iop.org/article/10.3847/1538-3881/ac18cb/meta
- "**TESS Eclipsing Binary Stars. I. Short Cadence Observations of 4584 Eclipsing Binaries Sectors 1-26**," A. Prsa, et al., arXiv:2110.13382 [astro-ph.SR], October 26, 2021. *
https://arxiv.org/abs/2110.13382

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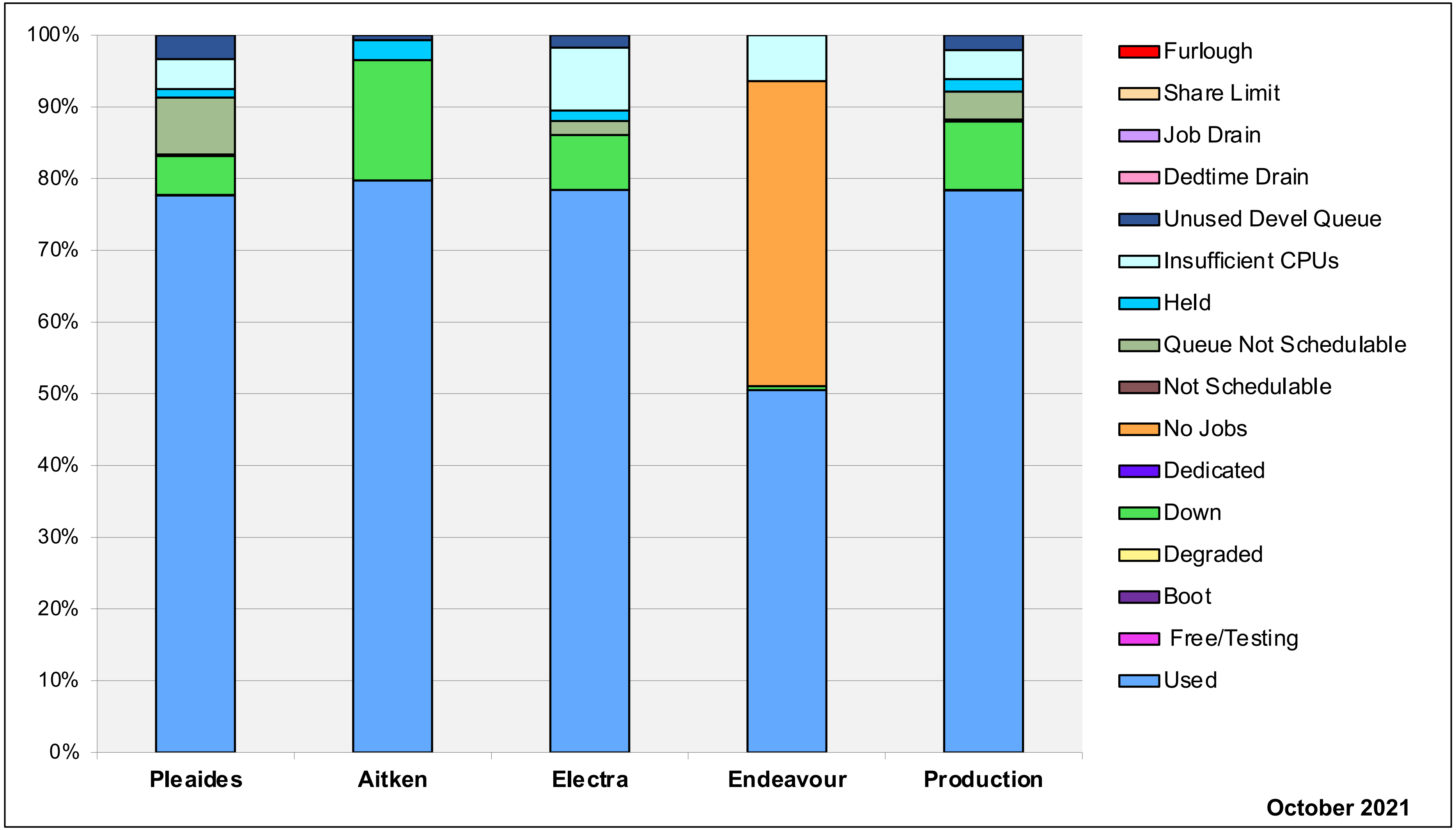
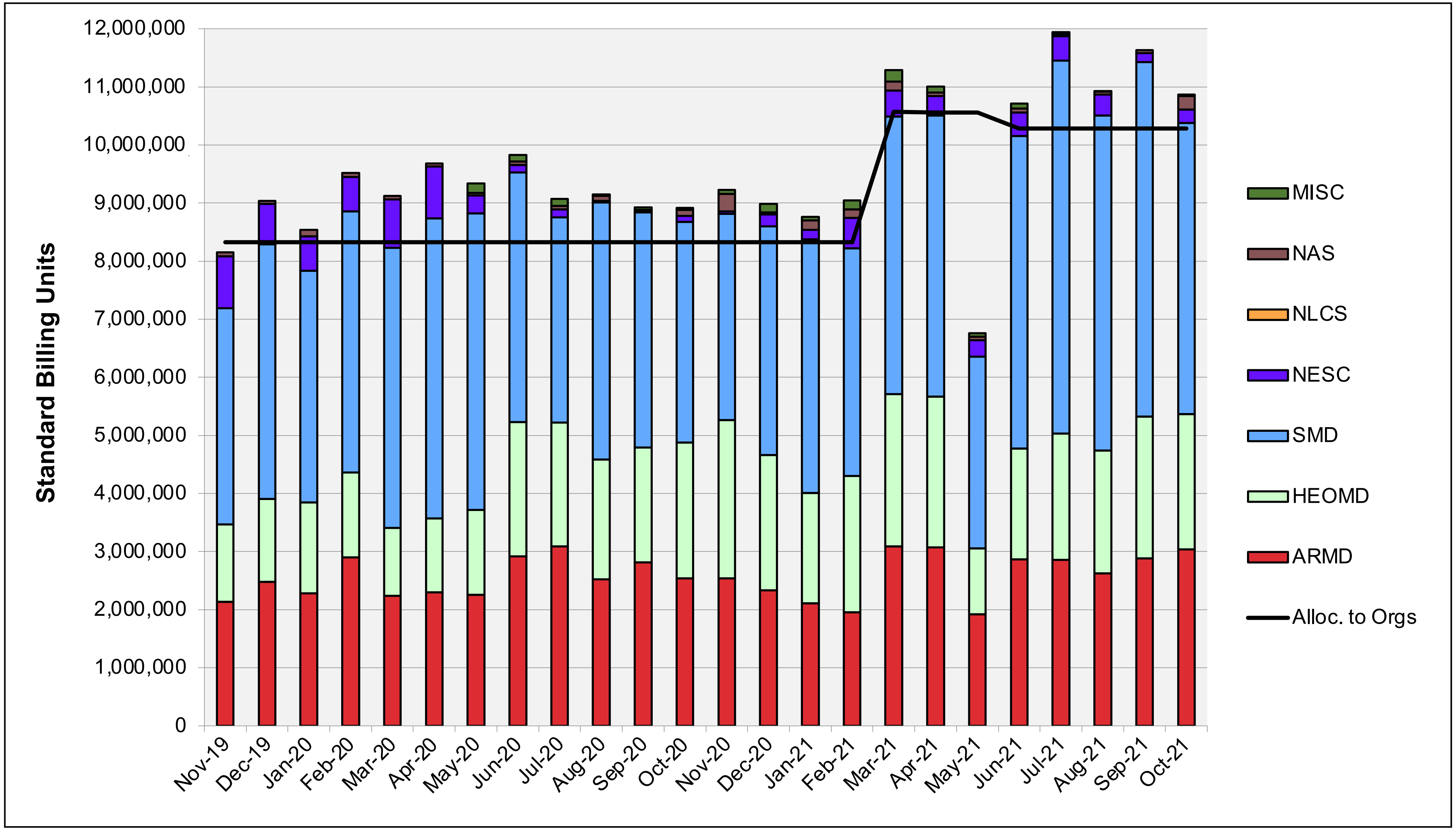
News and Events: Social Media

- **Coverage of NAS Stories**
  - Black Hole Merger Simulation (Throwback):
    - NAS: Twitter 6 retweets, 28 likes.
    - NASA Supercomputing: Facebook 162 users reached, 16 engagements, 5 likes, 2 shares.

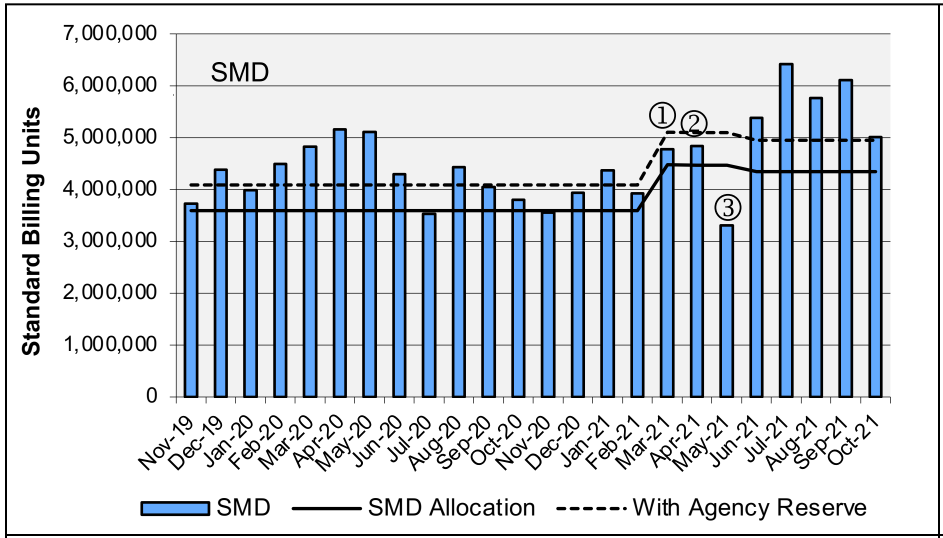
HECC Utilization

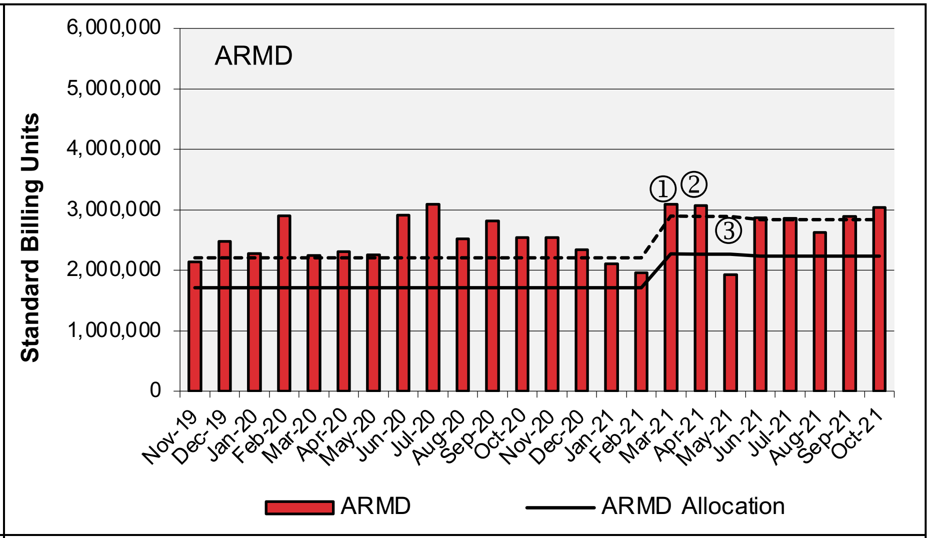


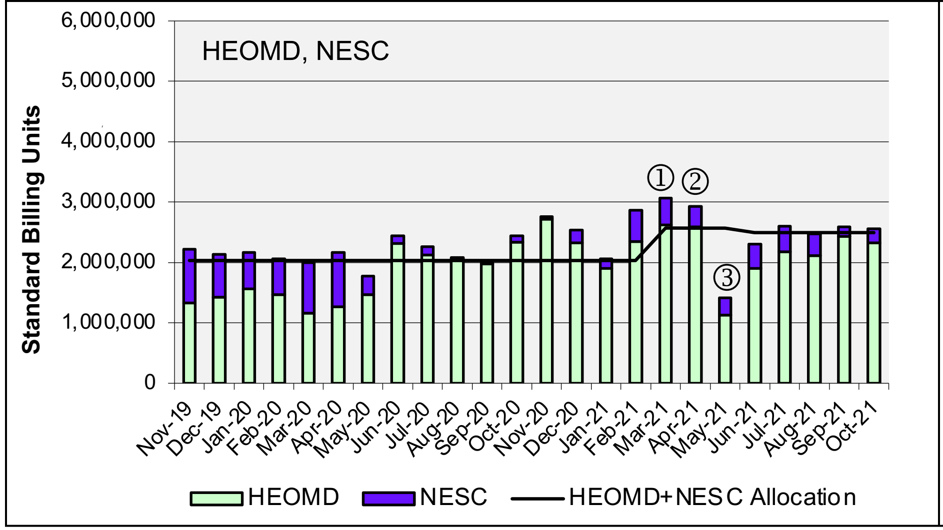
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month





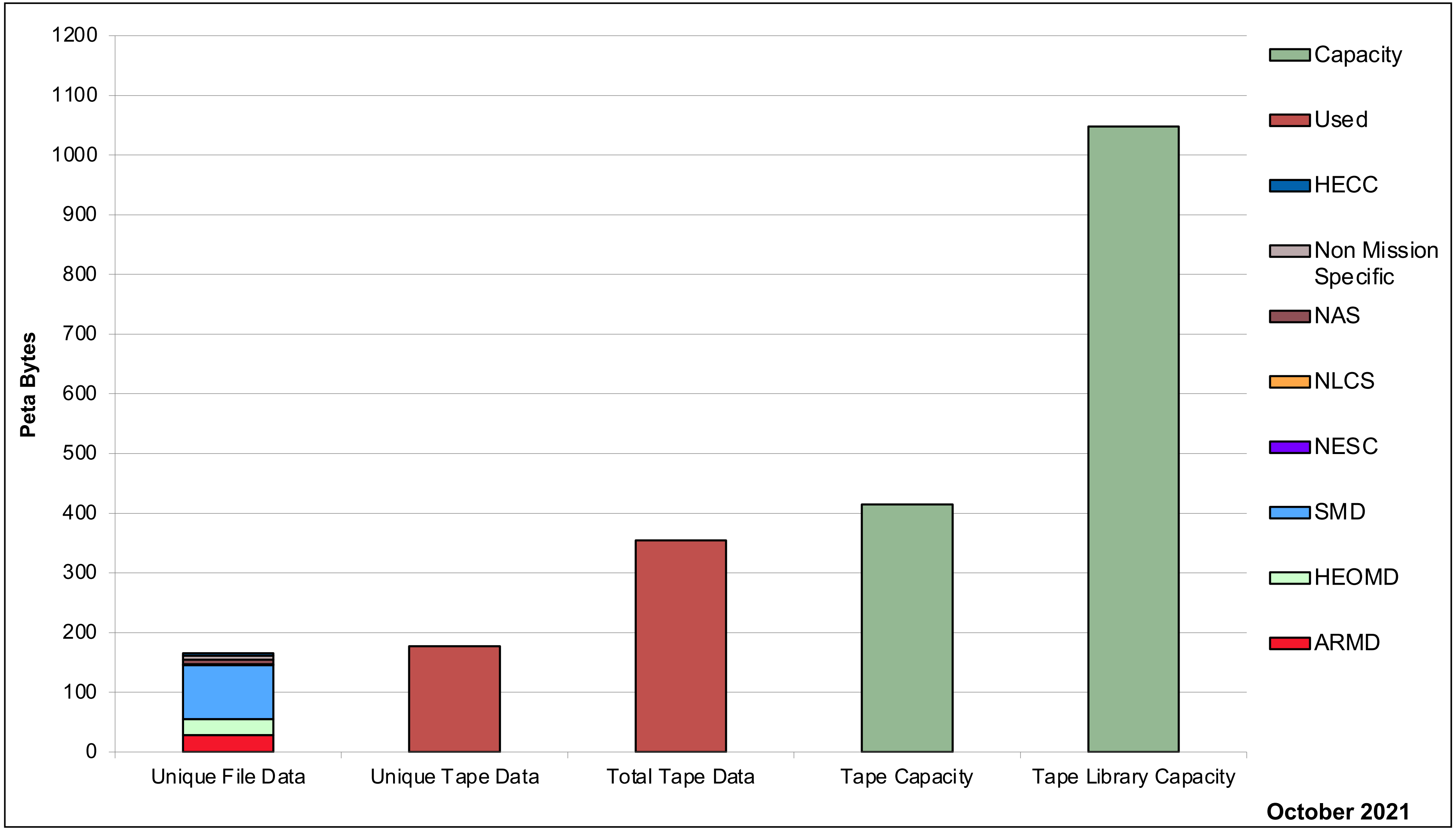


① 8 Rome Apollo racks introduced into Aitken

② Endeavour replaced with new hardware

③ Merope retired, Annual Maintenance

Tape Archive Status



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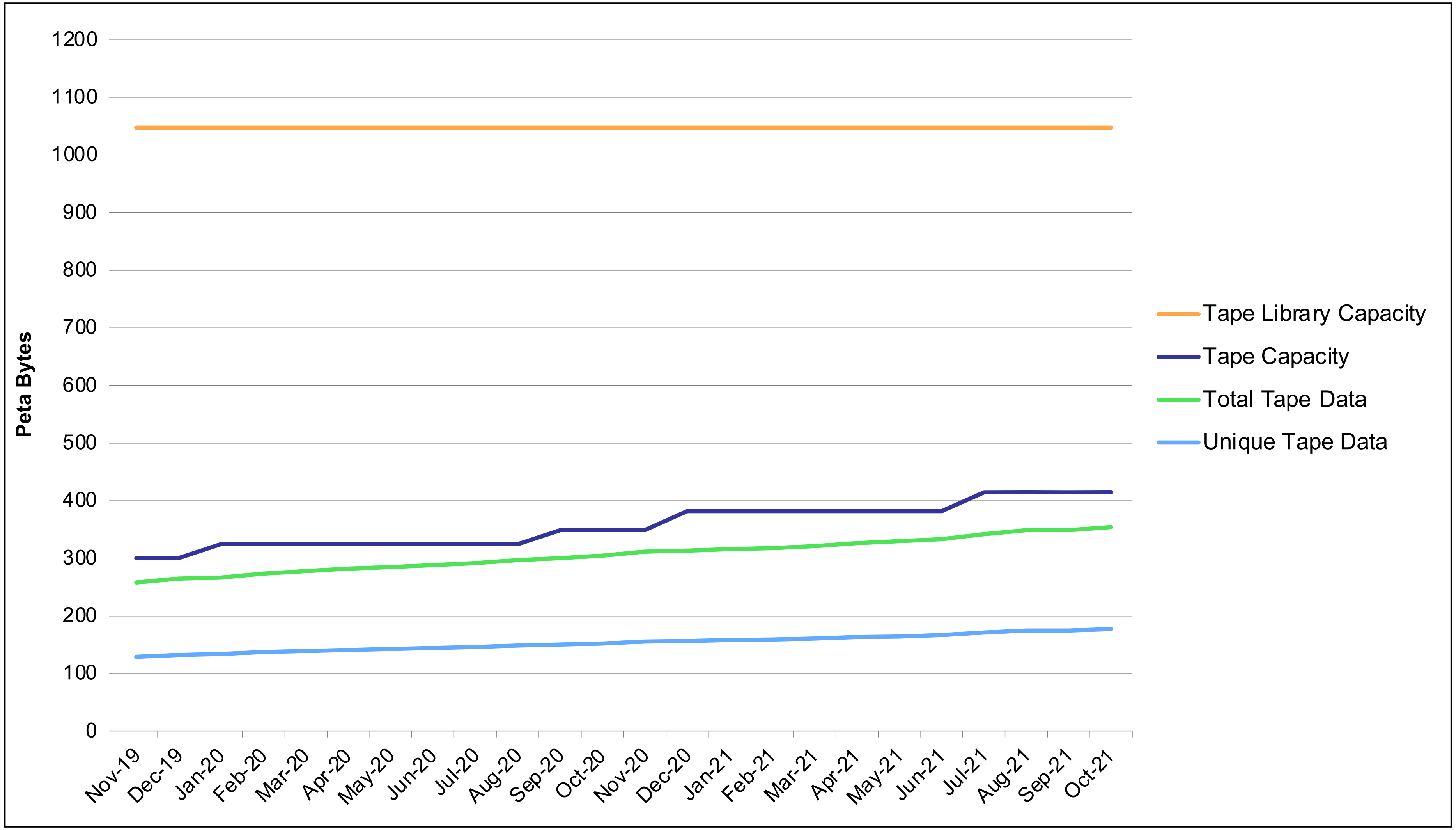
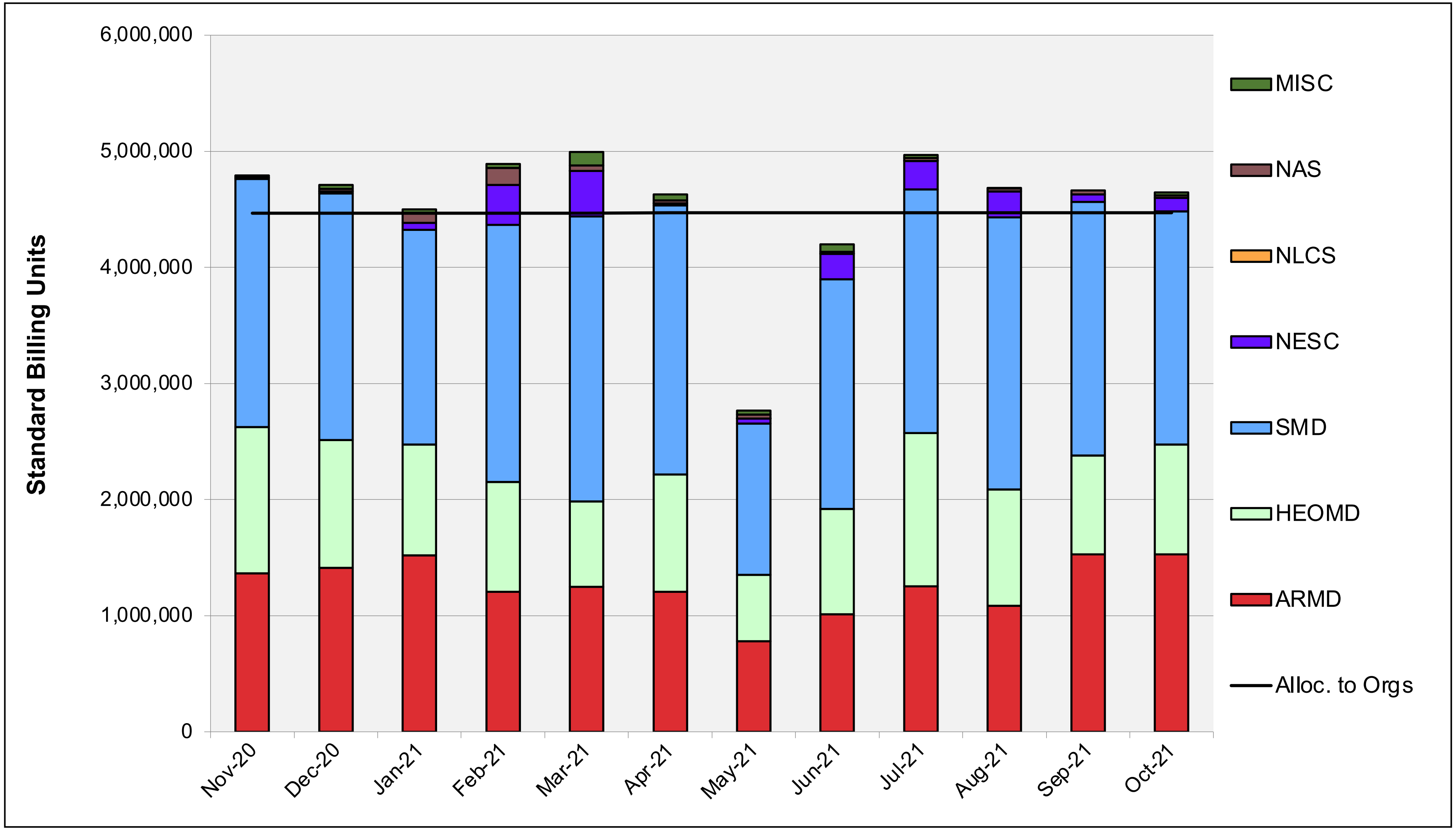
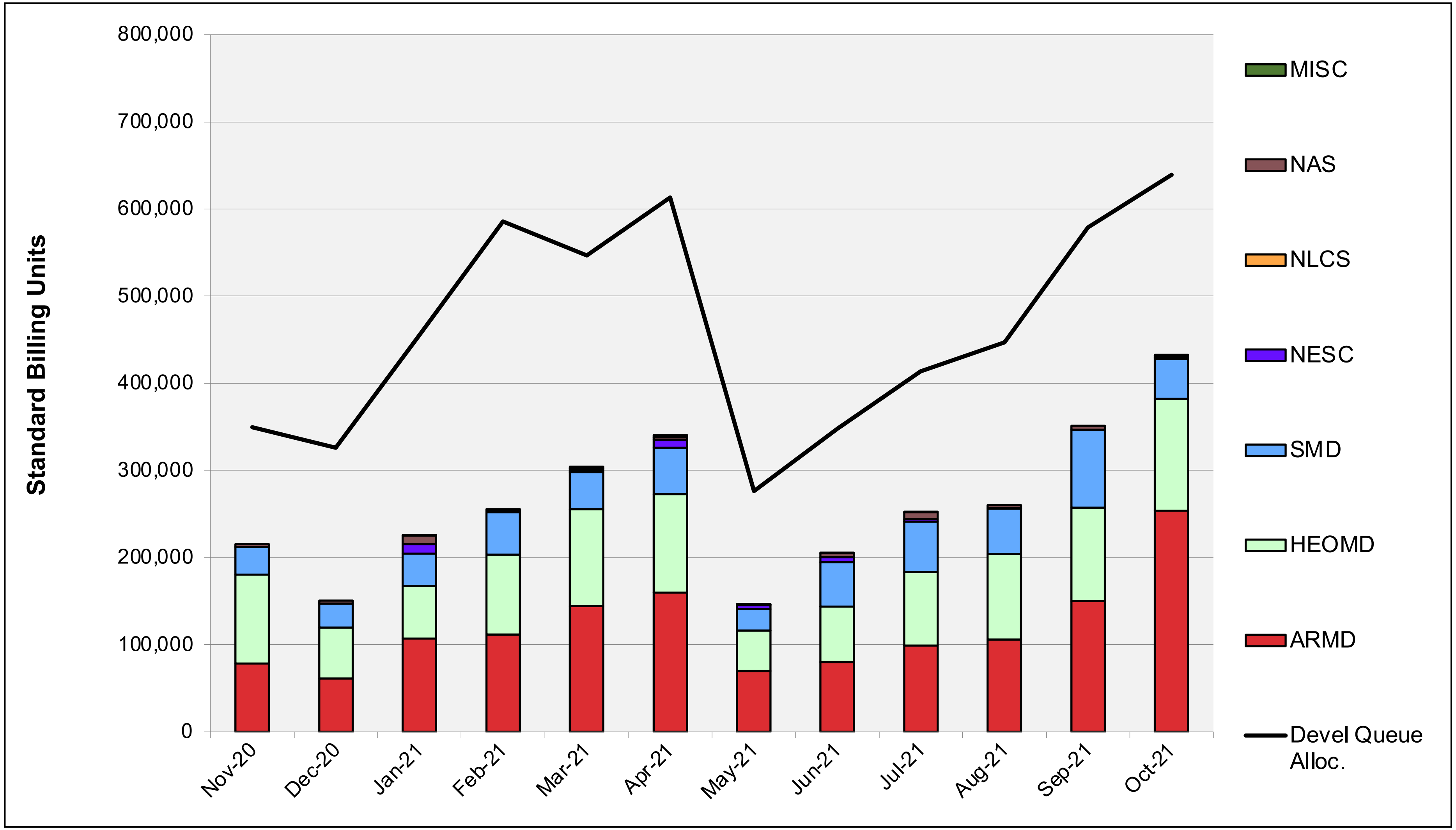


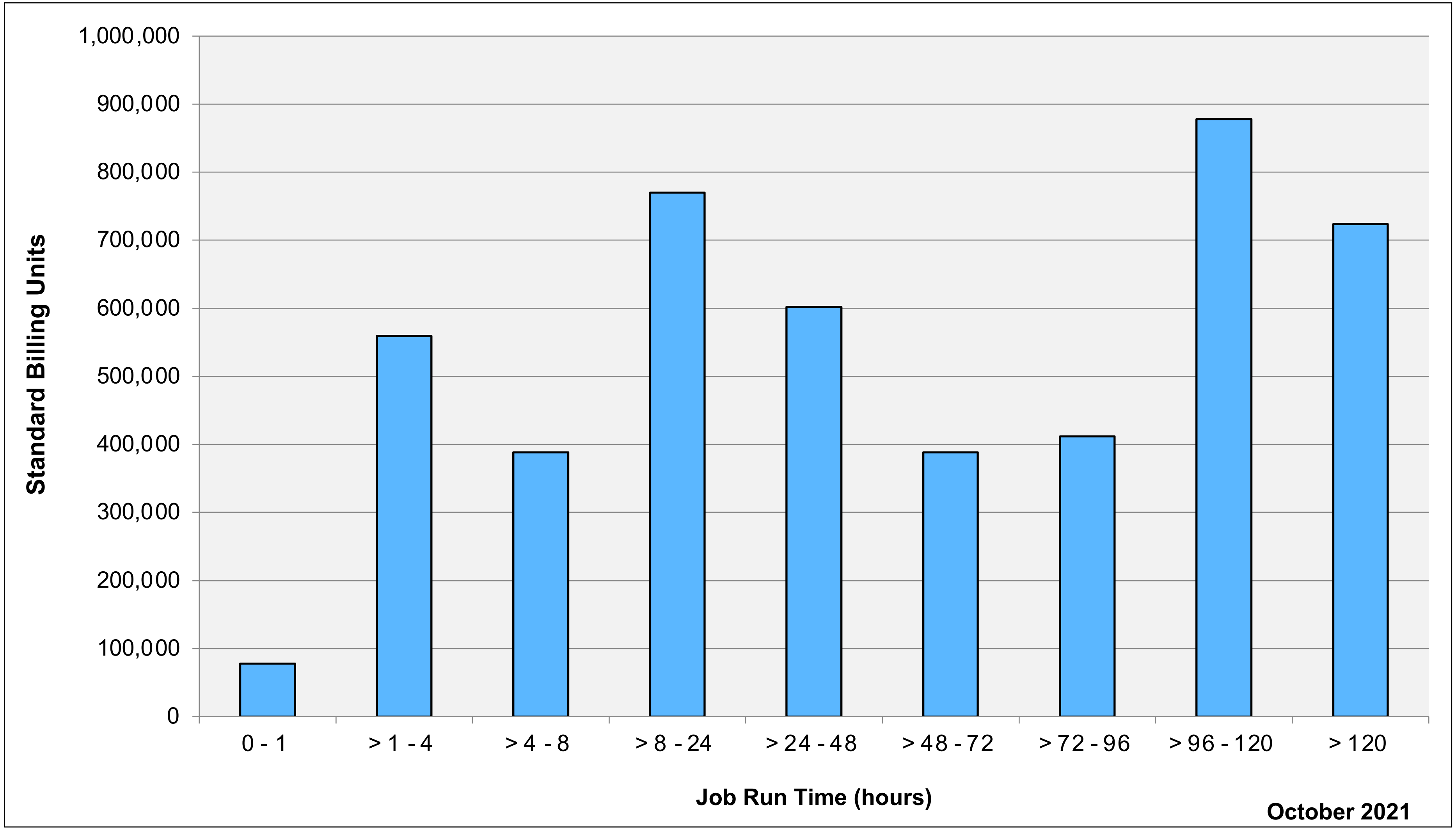
Pleiades: SBUs Reported, Normalized to 30-Day Month



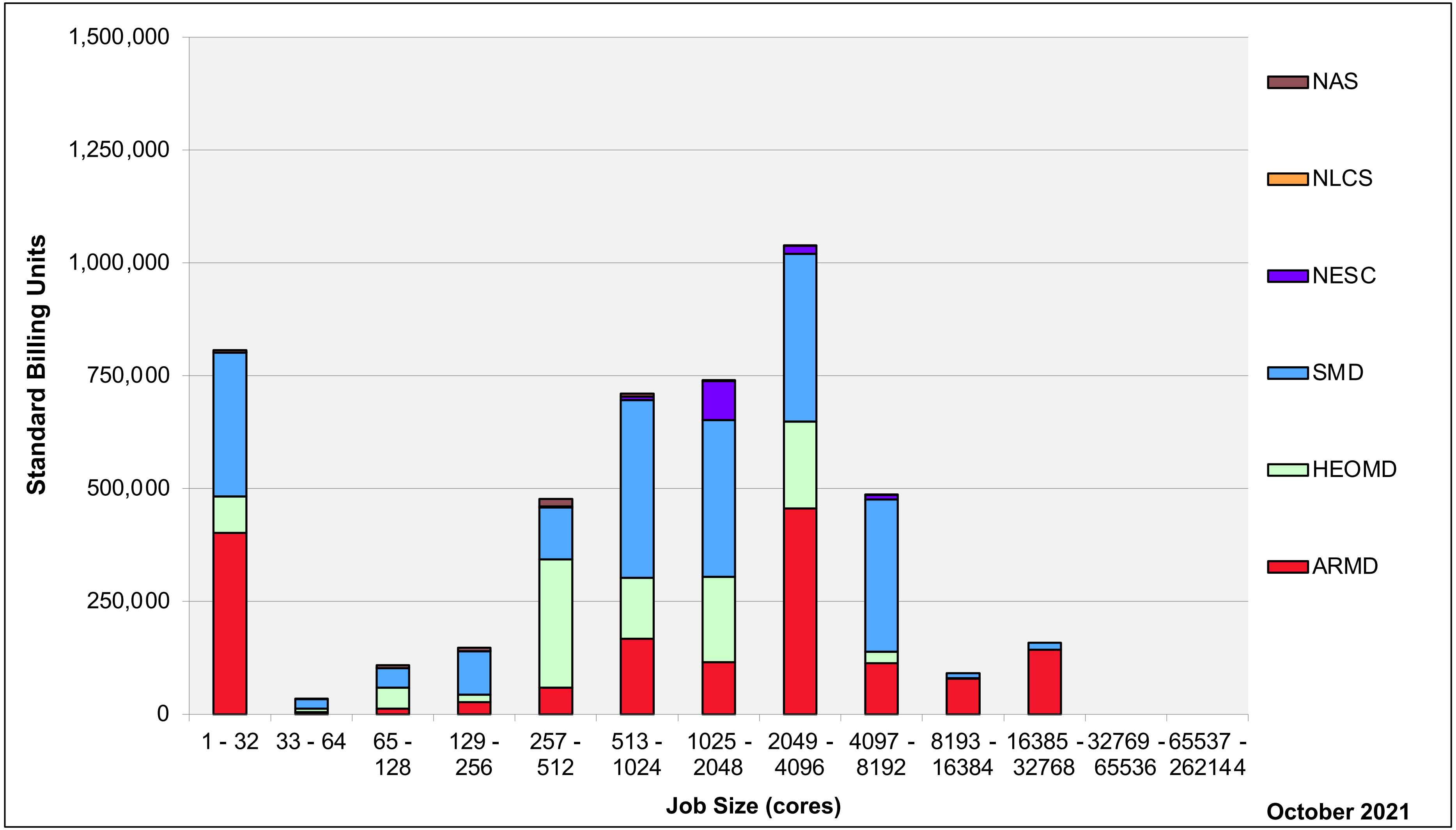
Pleiades: Devel Queue Utilization



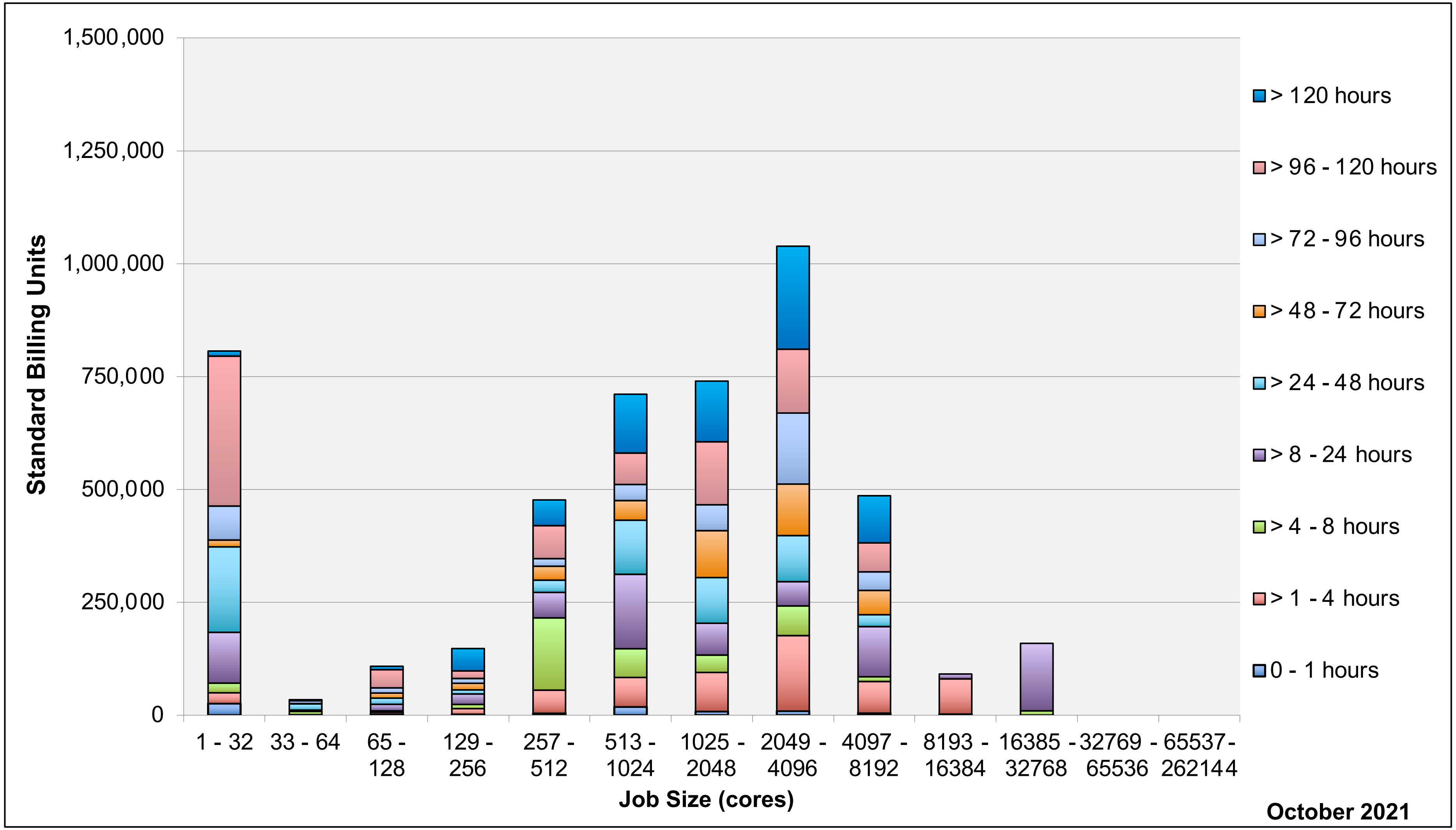
Pleiades: Monthly Utilization by Job Length



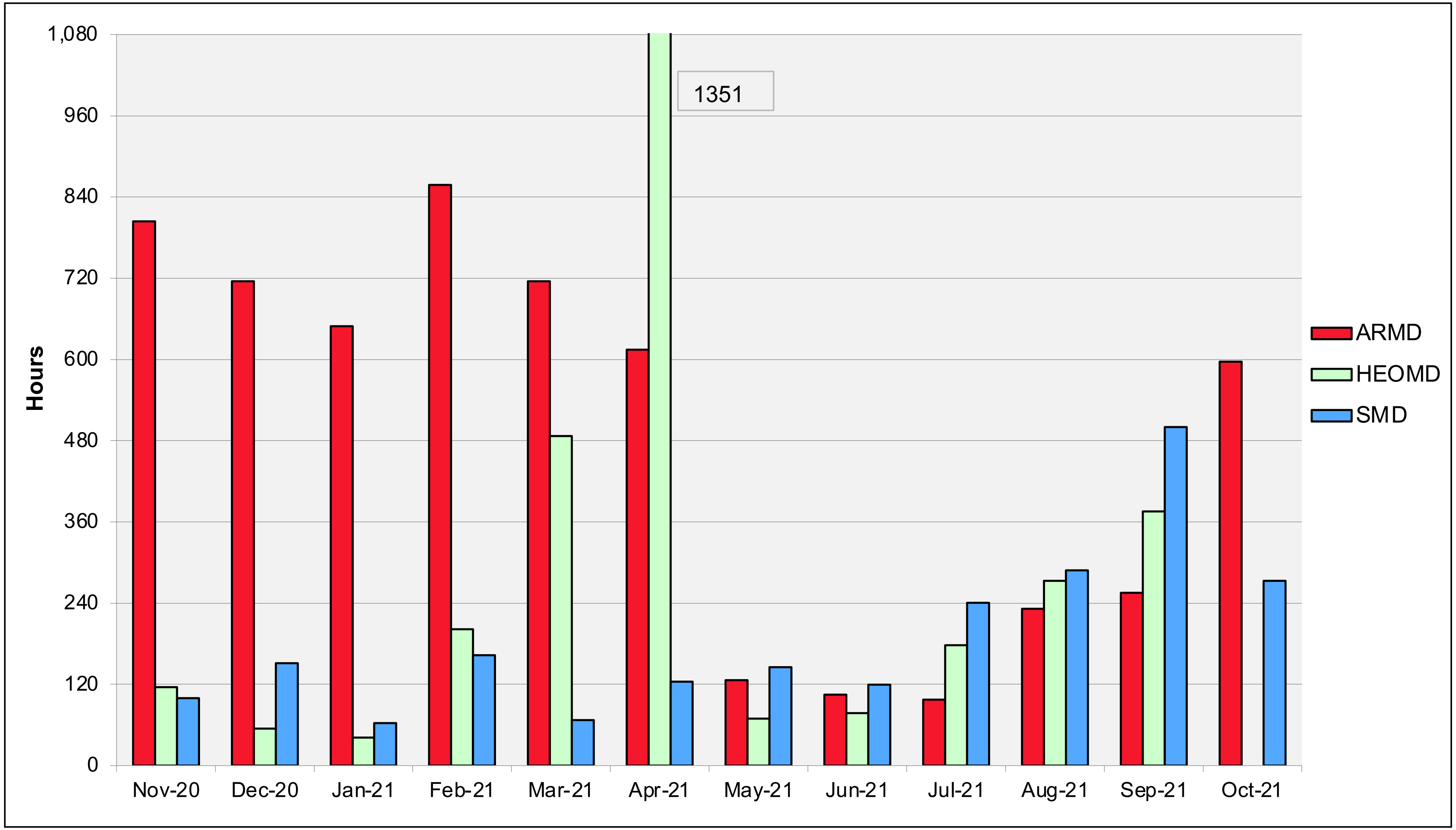
Pleiades: Monthly Utilization by Job Size



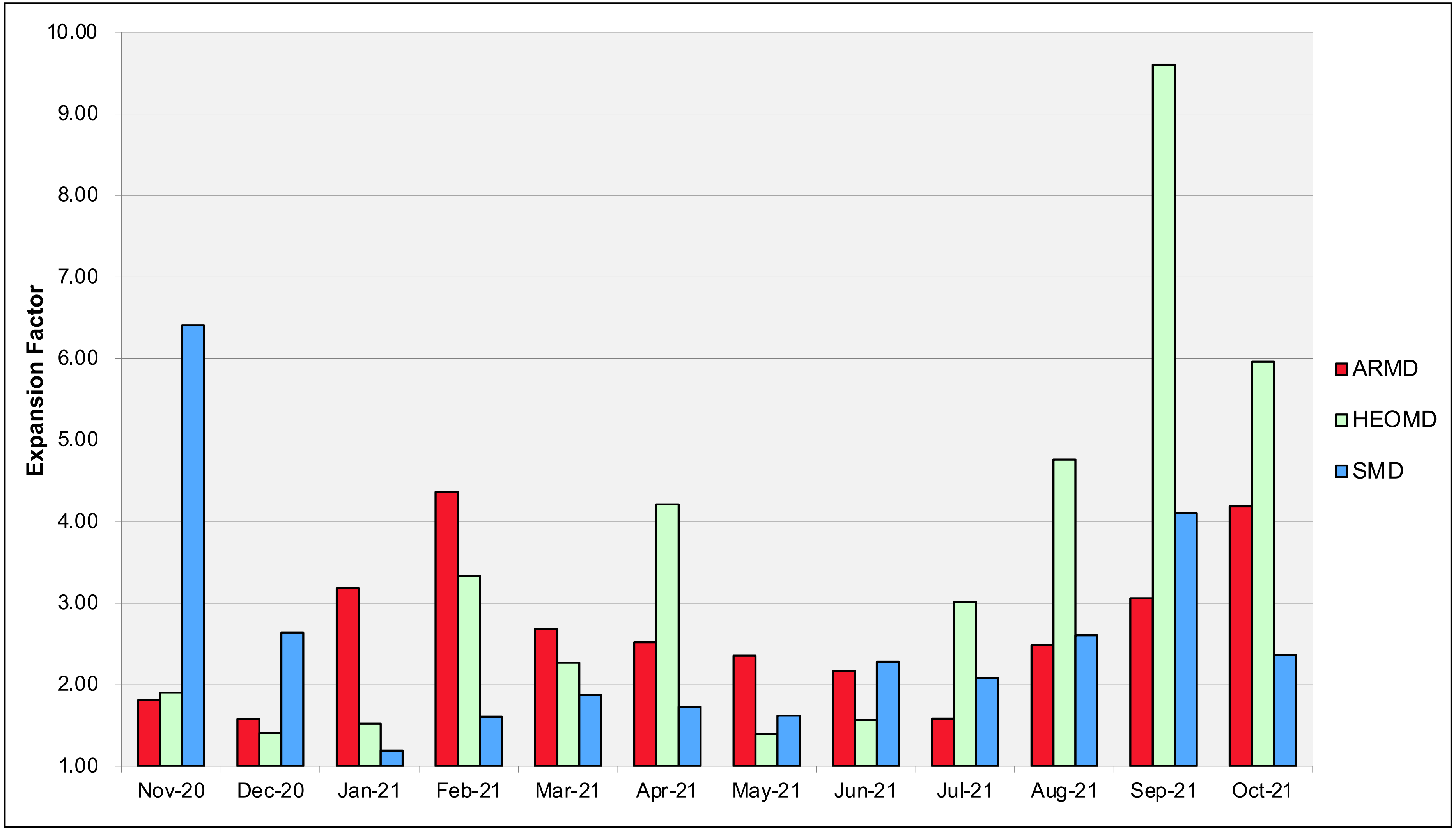
Pleiades: Monthly Utilization by Size and Length



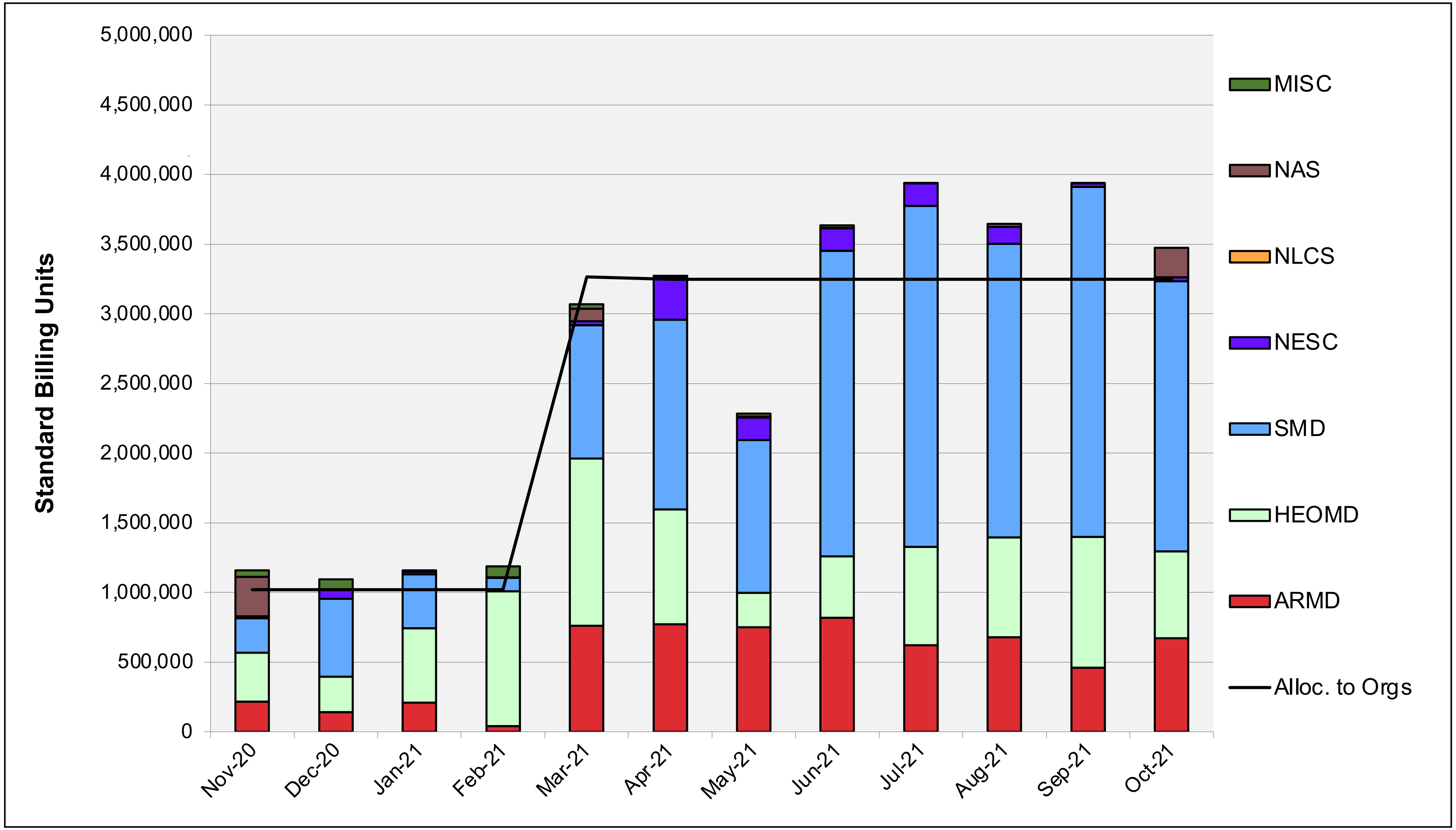
Pleiades: Average Time to Clear All Jobs



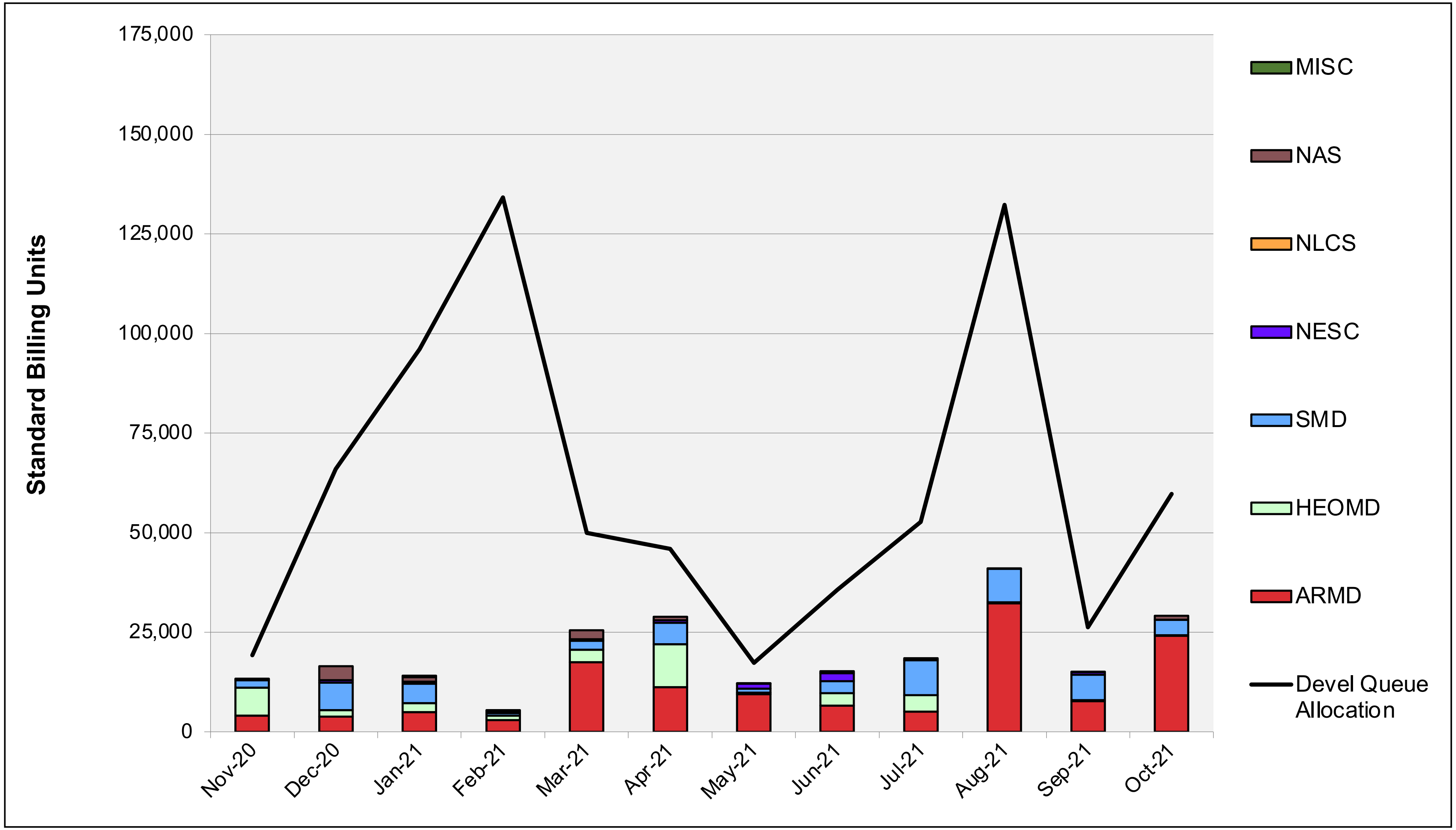
Pleiades: Average Expansion Factor



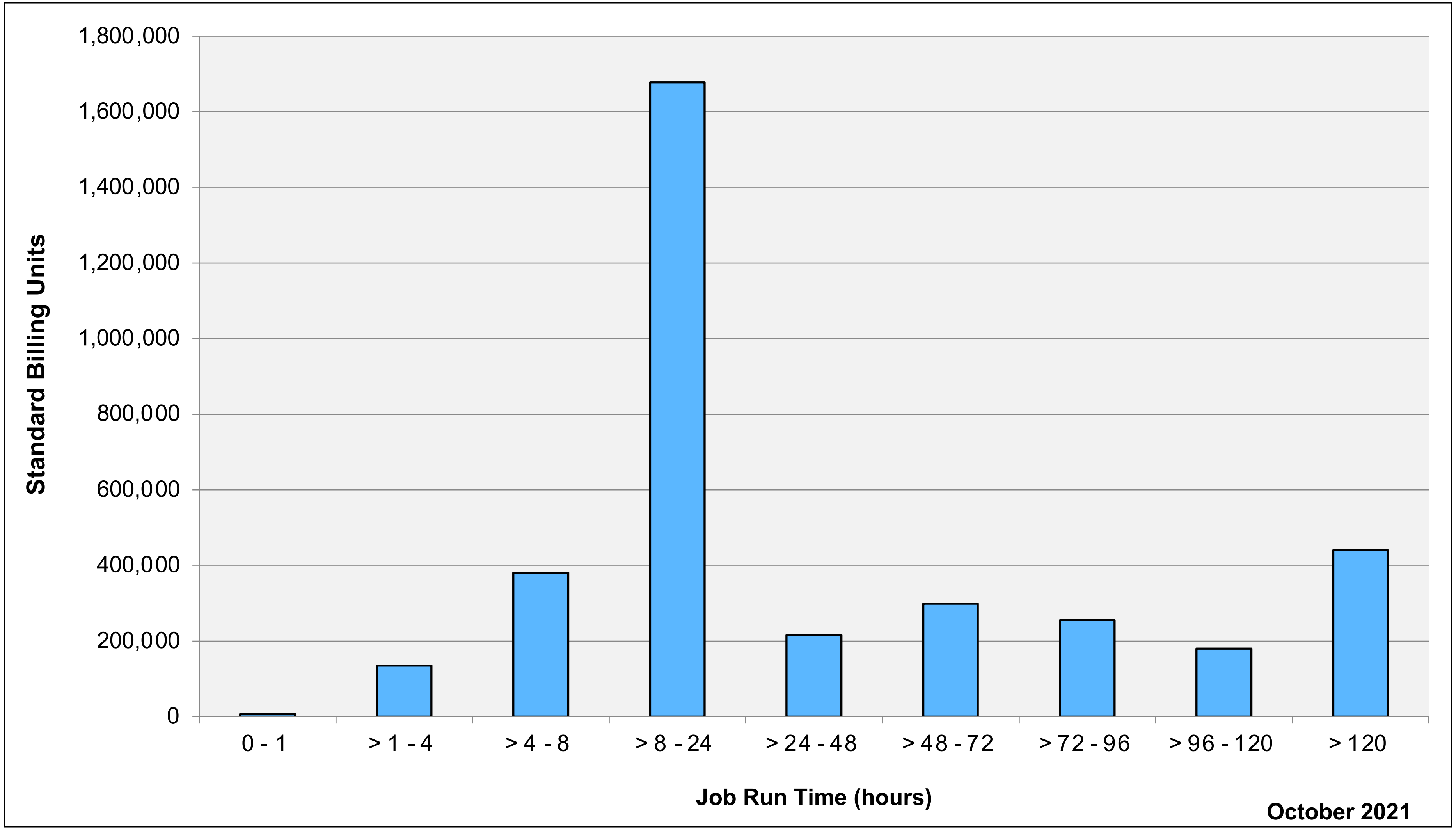
Aitken: SBUs Reported, Normalized to 30-Day Month



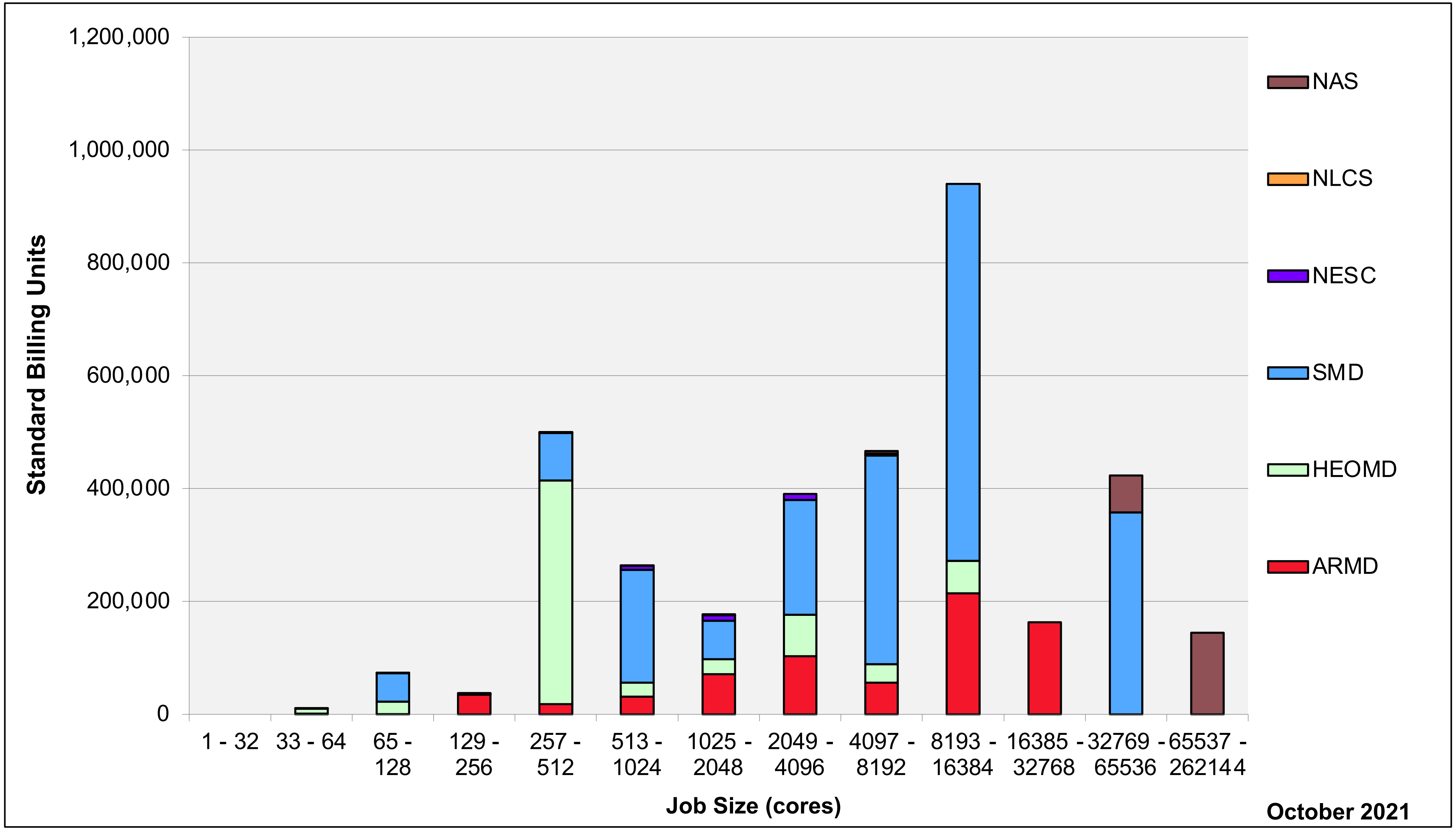
Aitken: Devel Queue Utilization



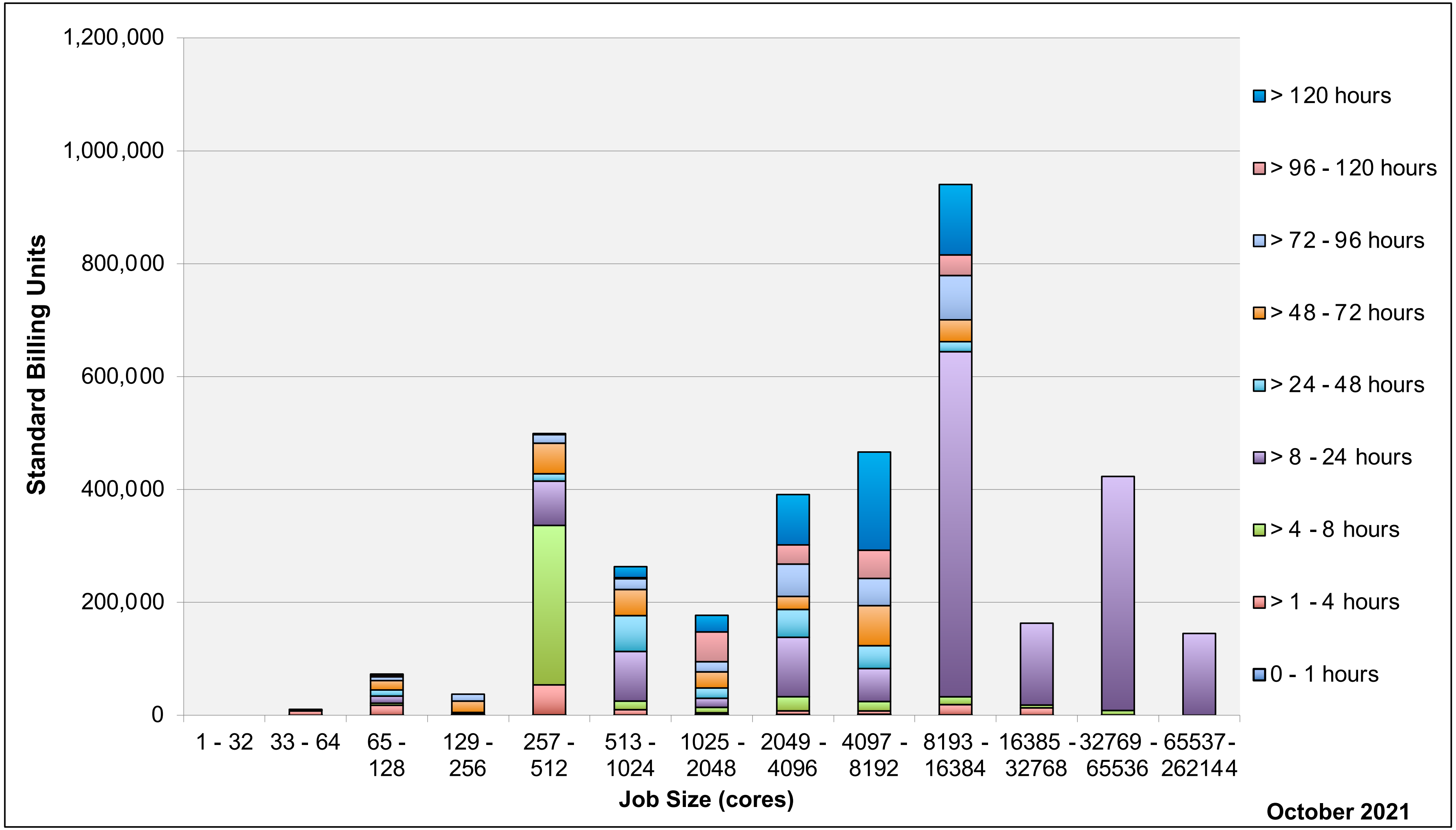
Aitken: Monthly Utilization by Job Length



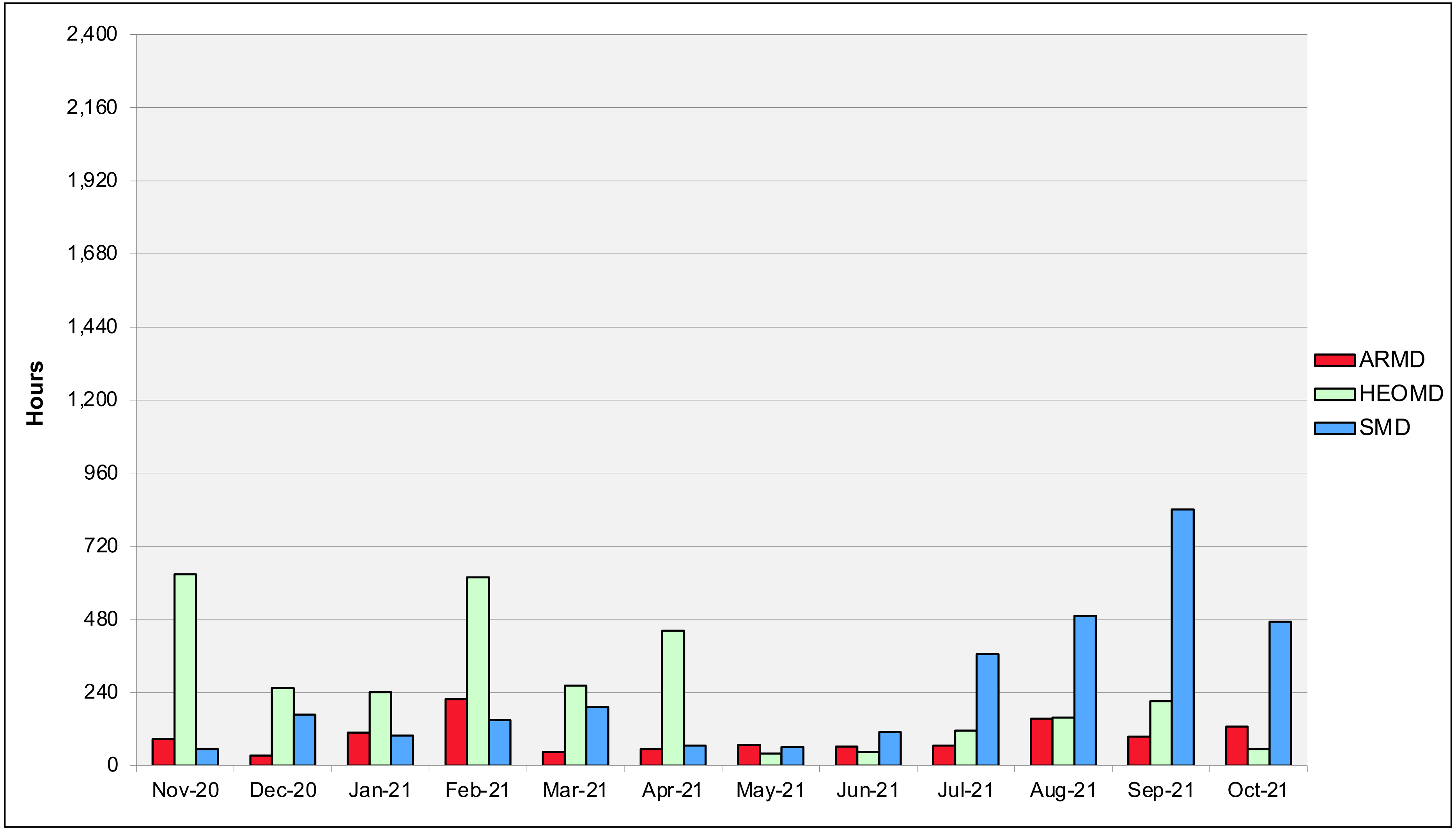
Aitken: Monthly Utilization by Job Size



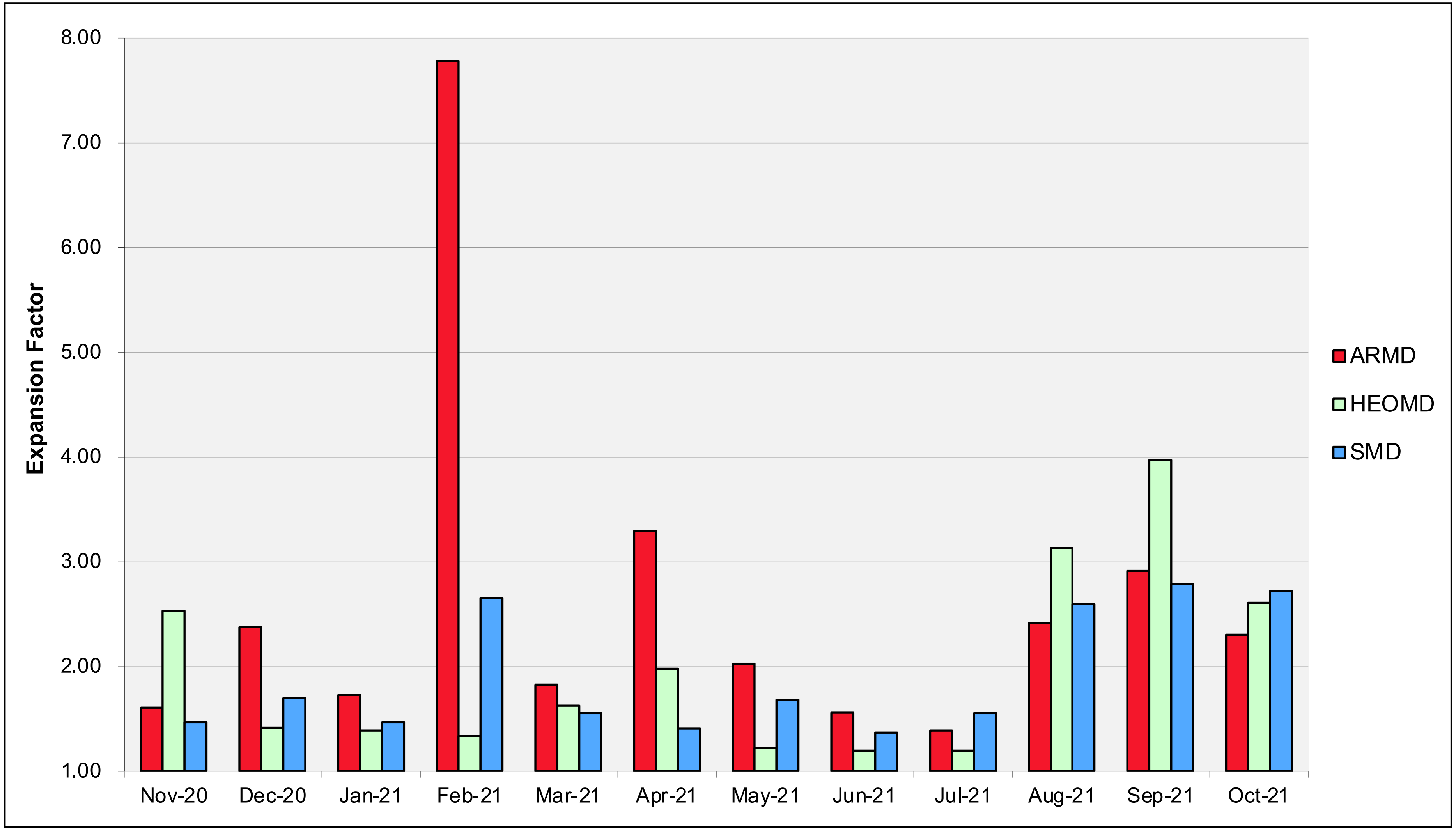
Aitken: Monthly Utilization by Size and Length



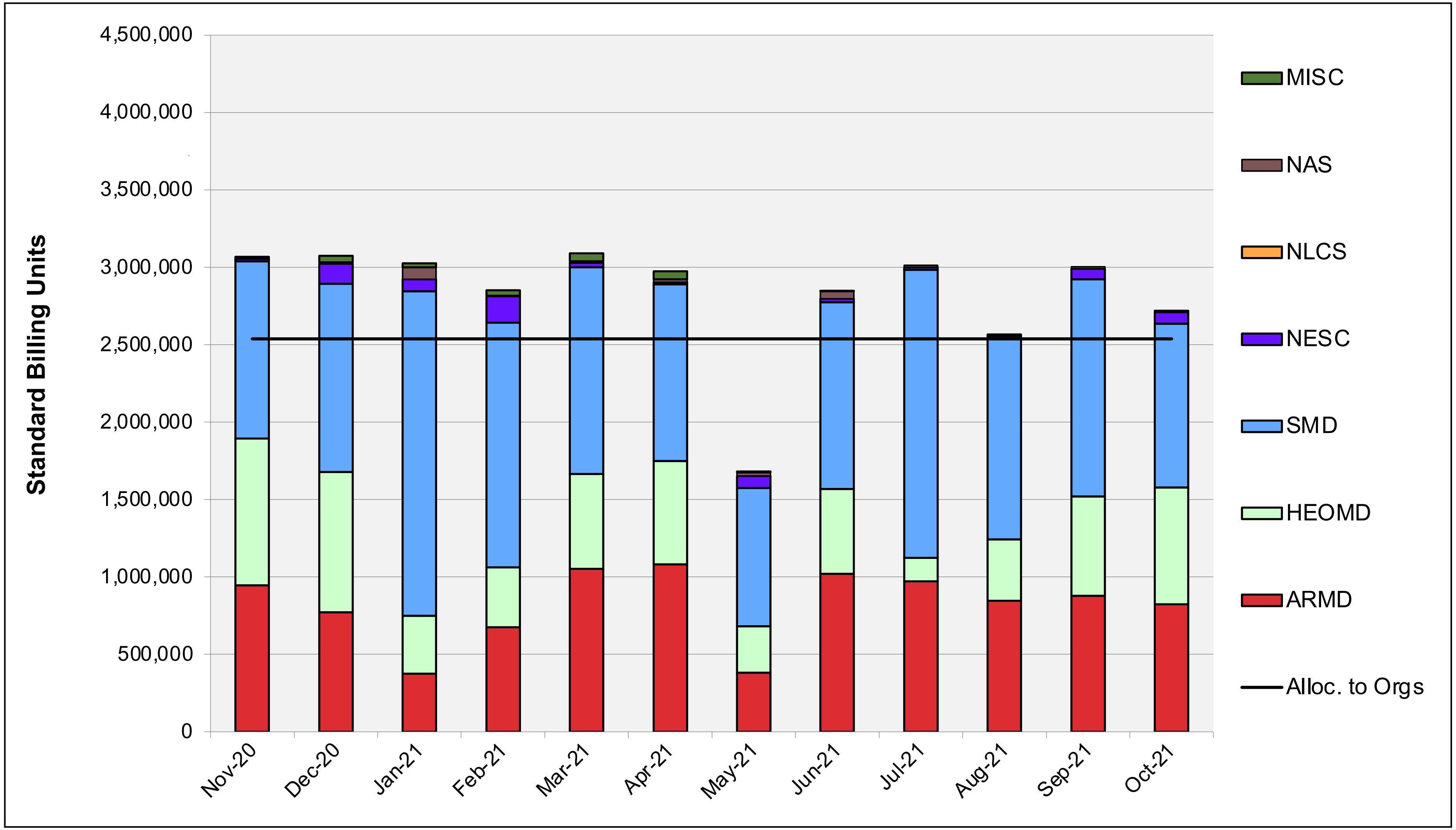
Aitken: Average Time to Clear All Jobs



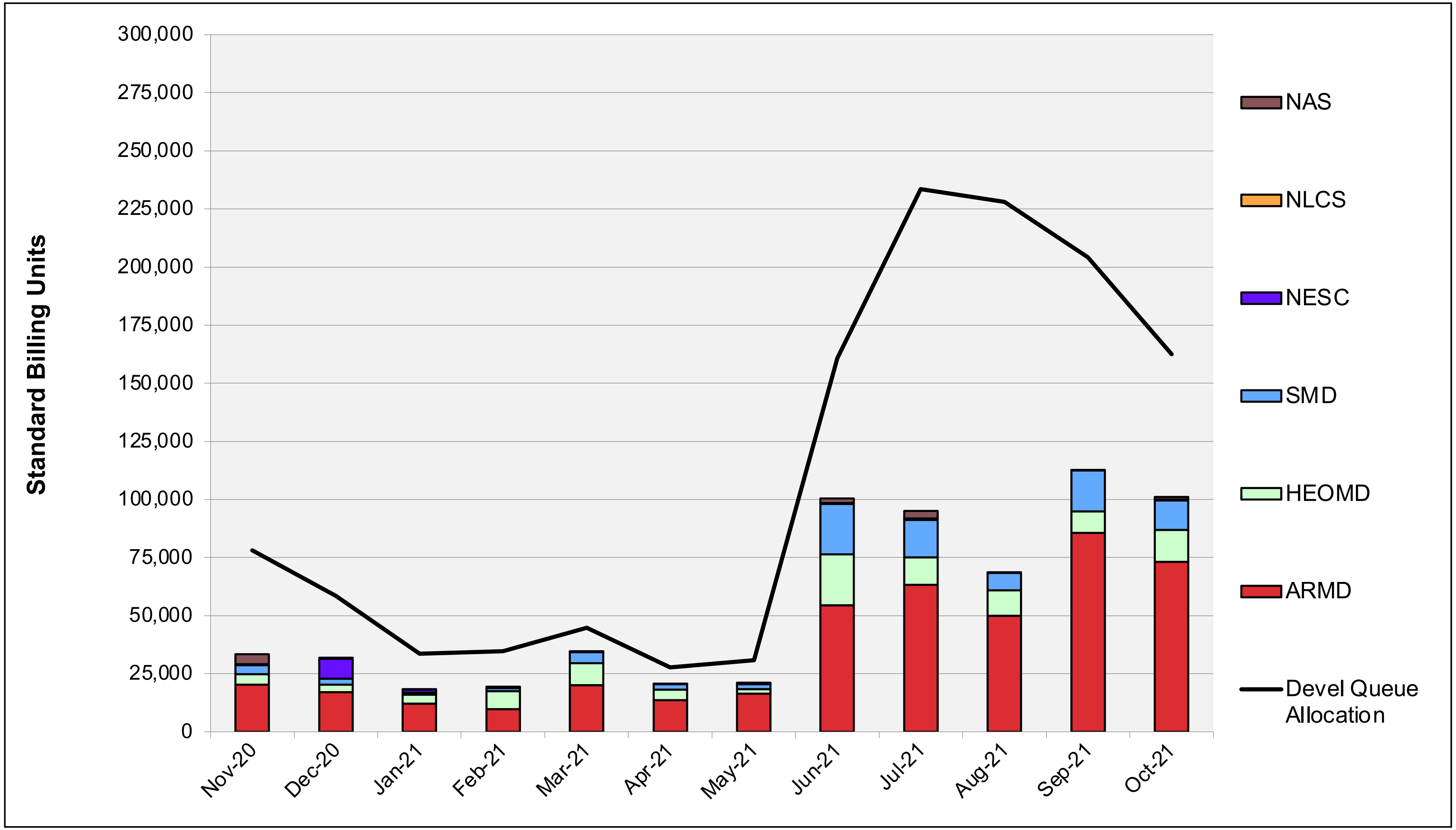
Aitken: Average Expansion Factor



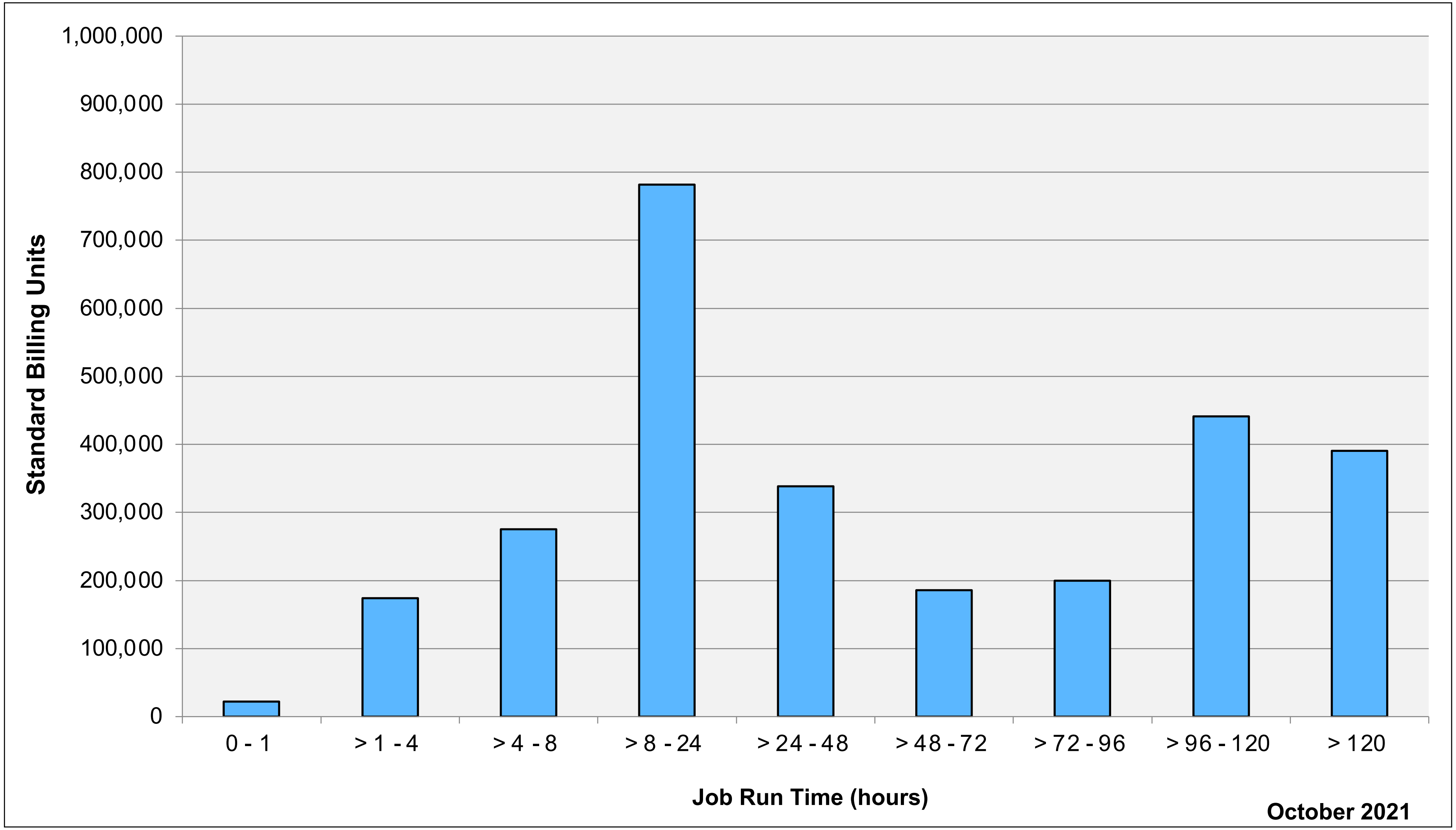
Electra: SBUs Reported, Normalized to 30-Day Month



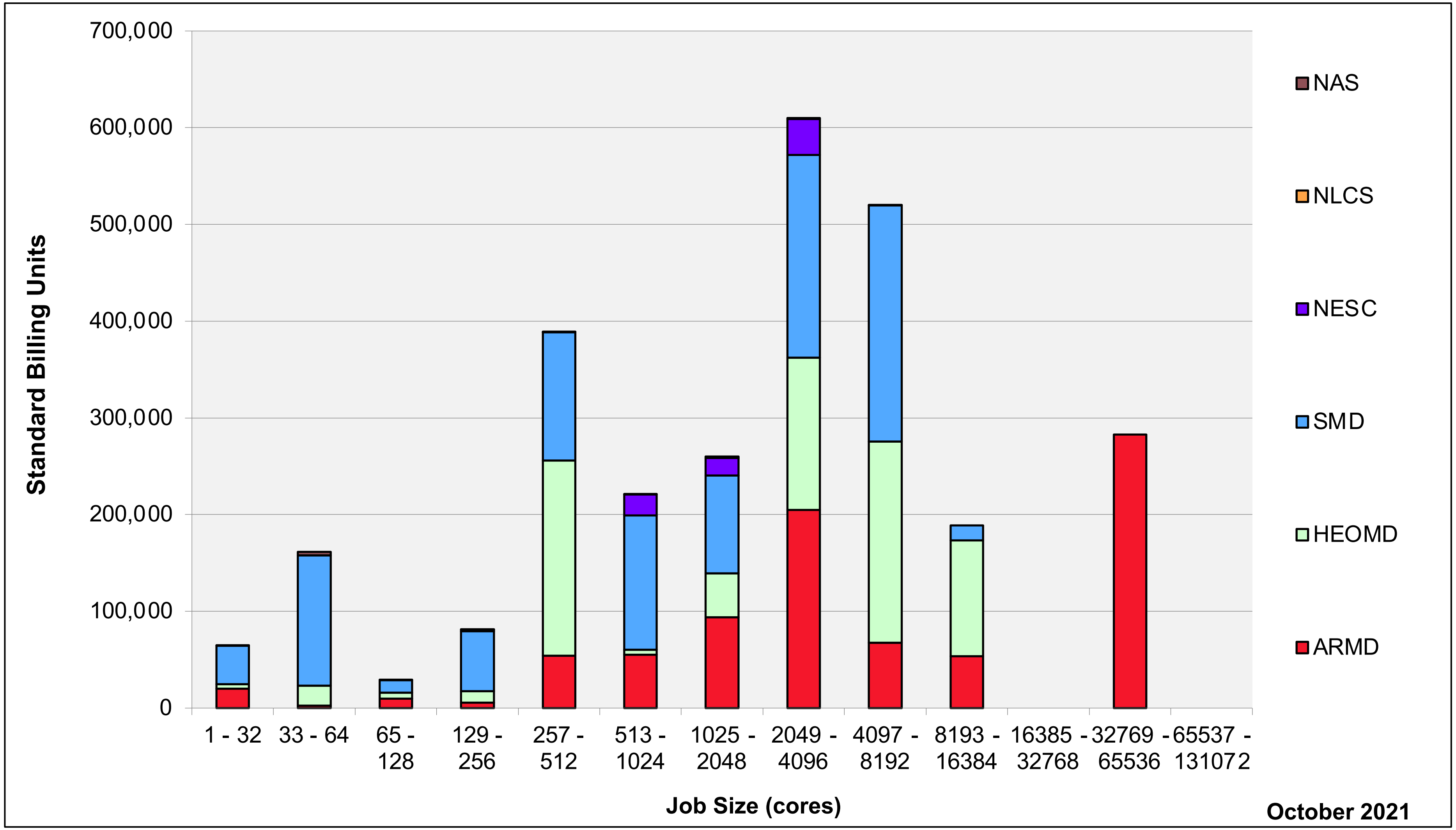
Electra: Devel Queue Utilization



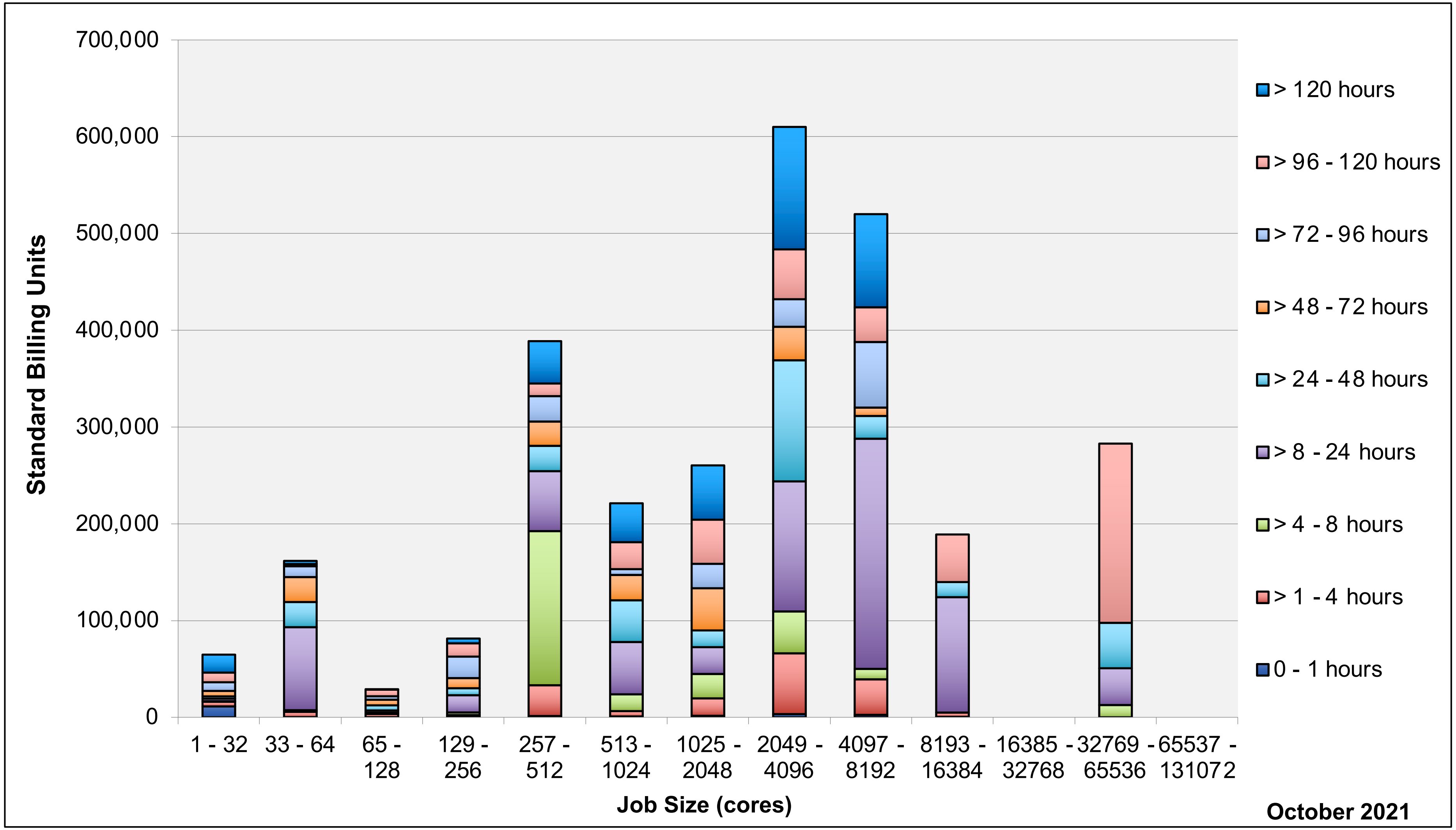
Electra: Monthly Utilization by Job Length



Electra: Monthly Utilization by Job Size



Electra: Monthly Utilization by Size and Length



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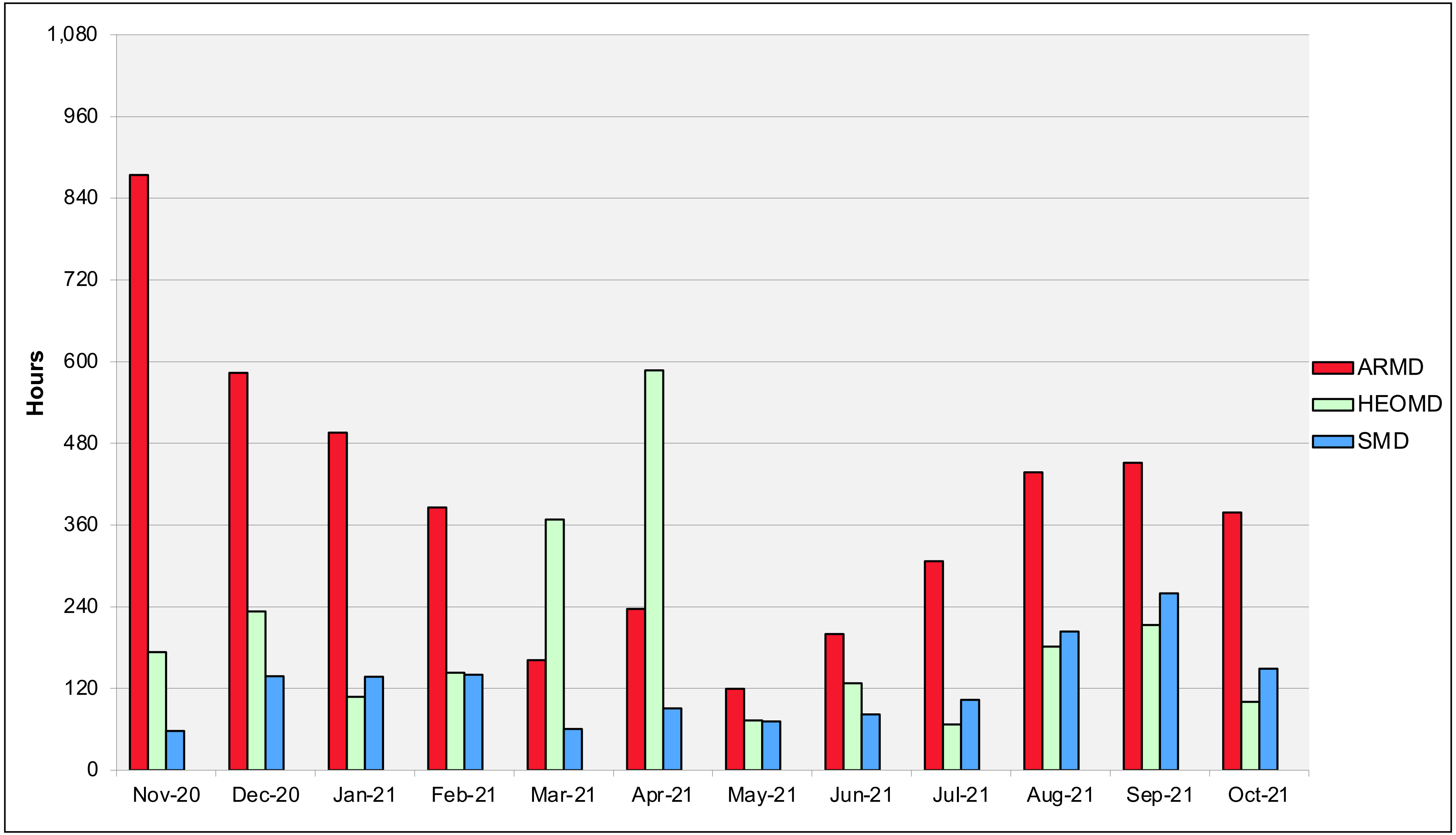
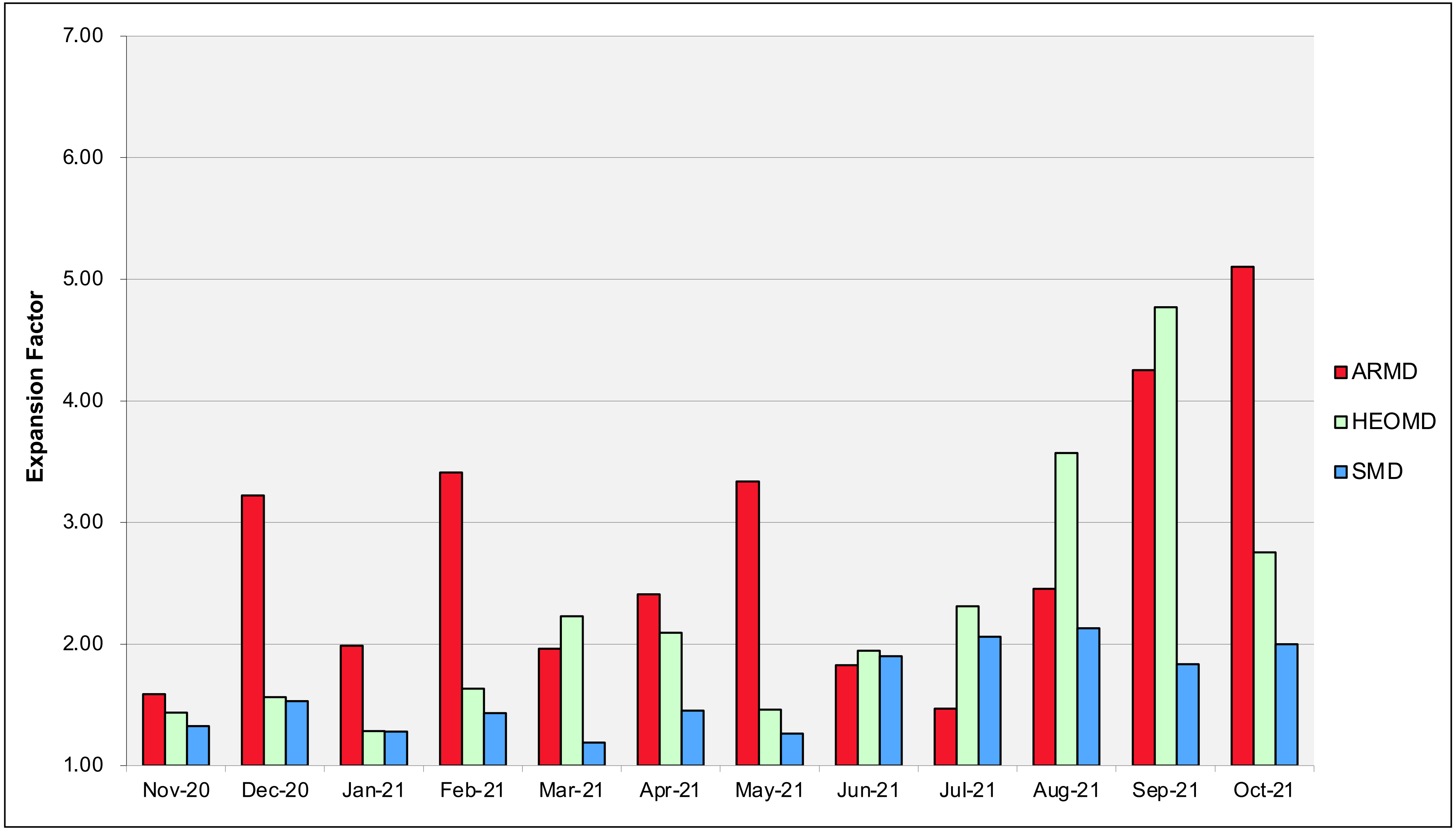
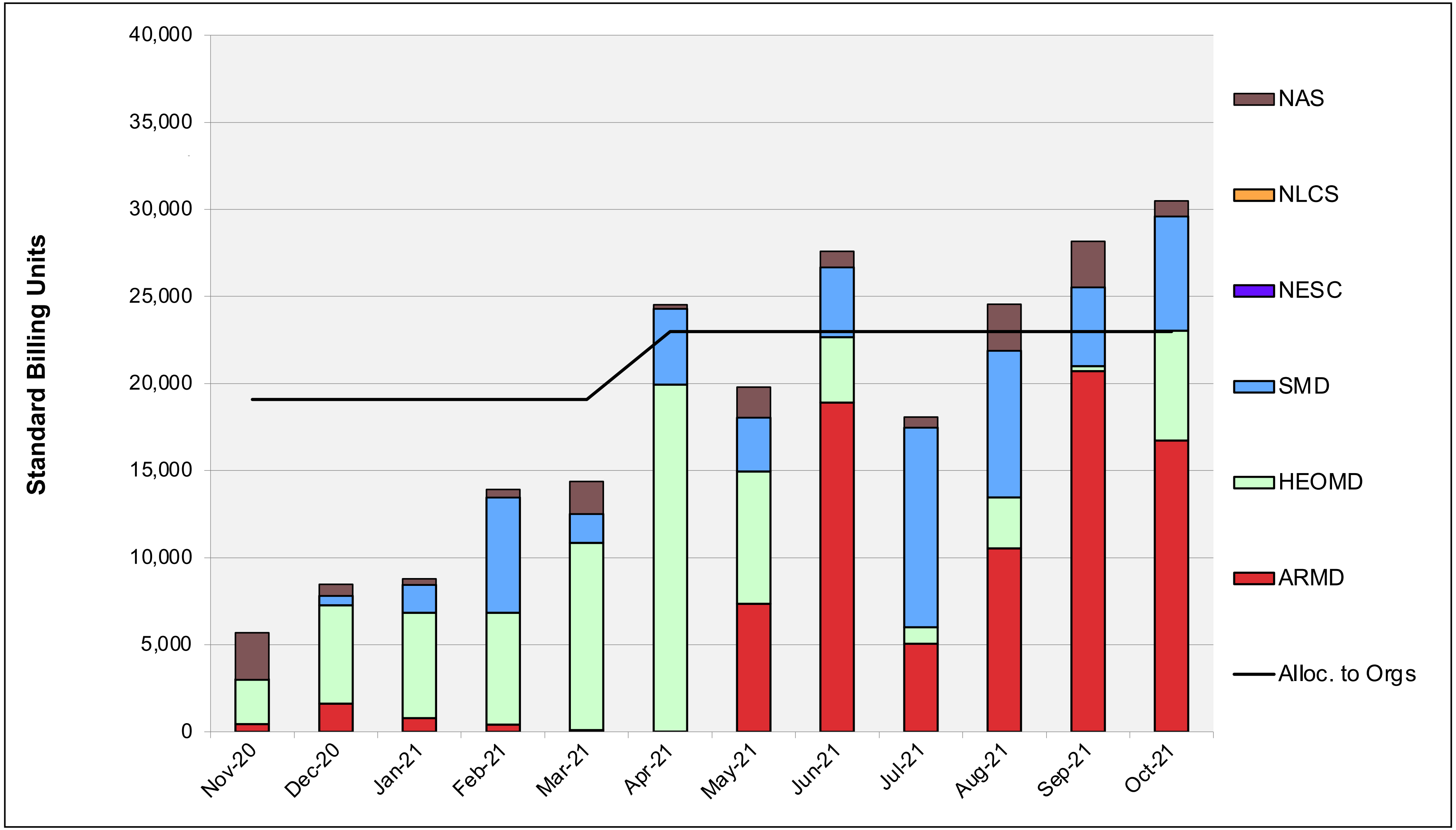


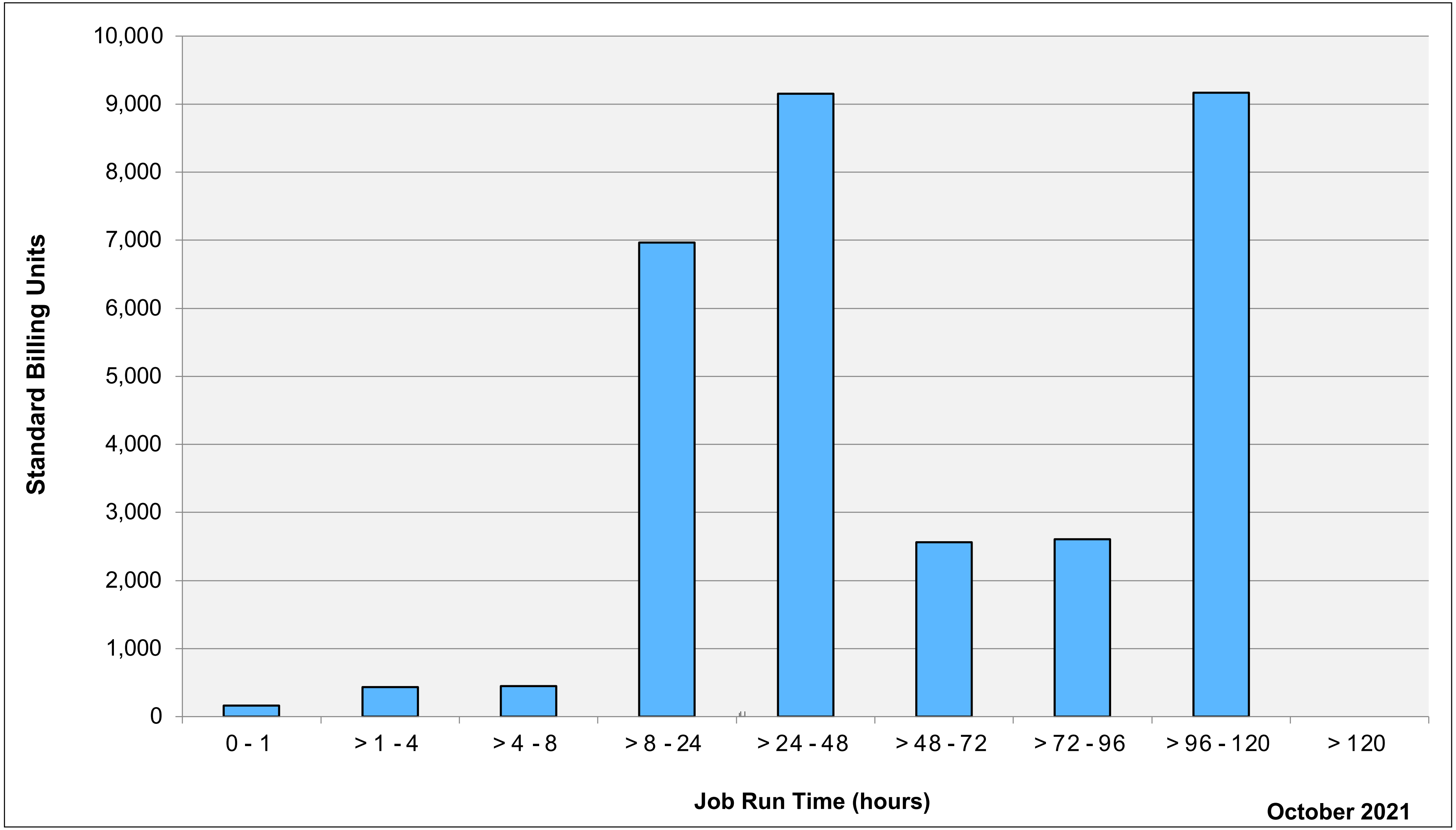
Electra: Average Expansion Factor



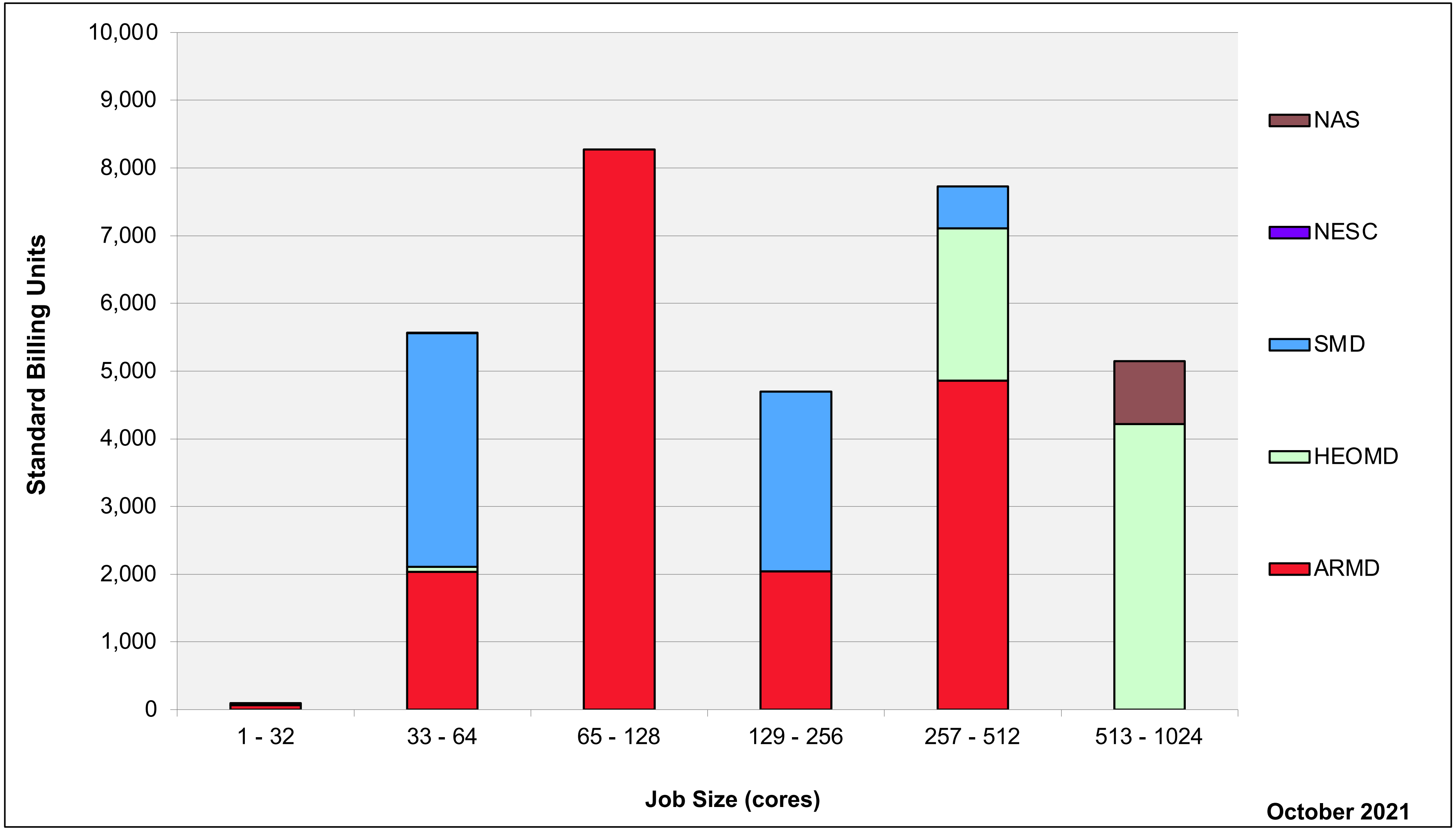
Endeavour: SBUs Reported, Normalized to 30-Day Month



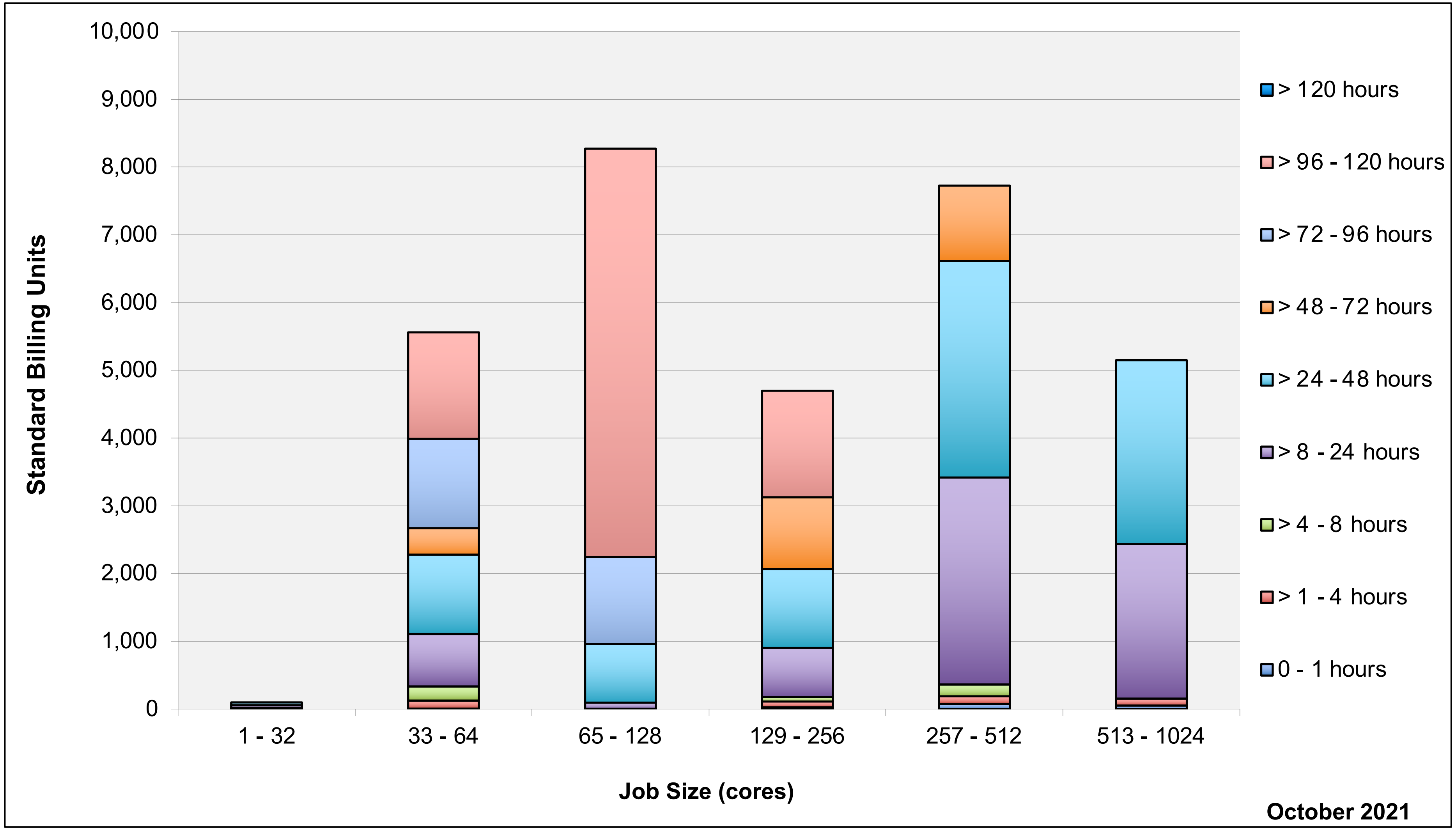
Endeavour: Monthly Utilization by Job Length



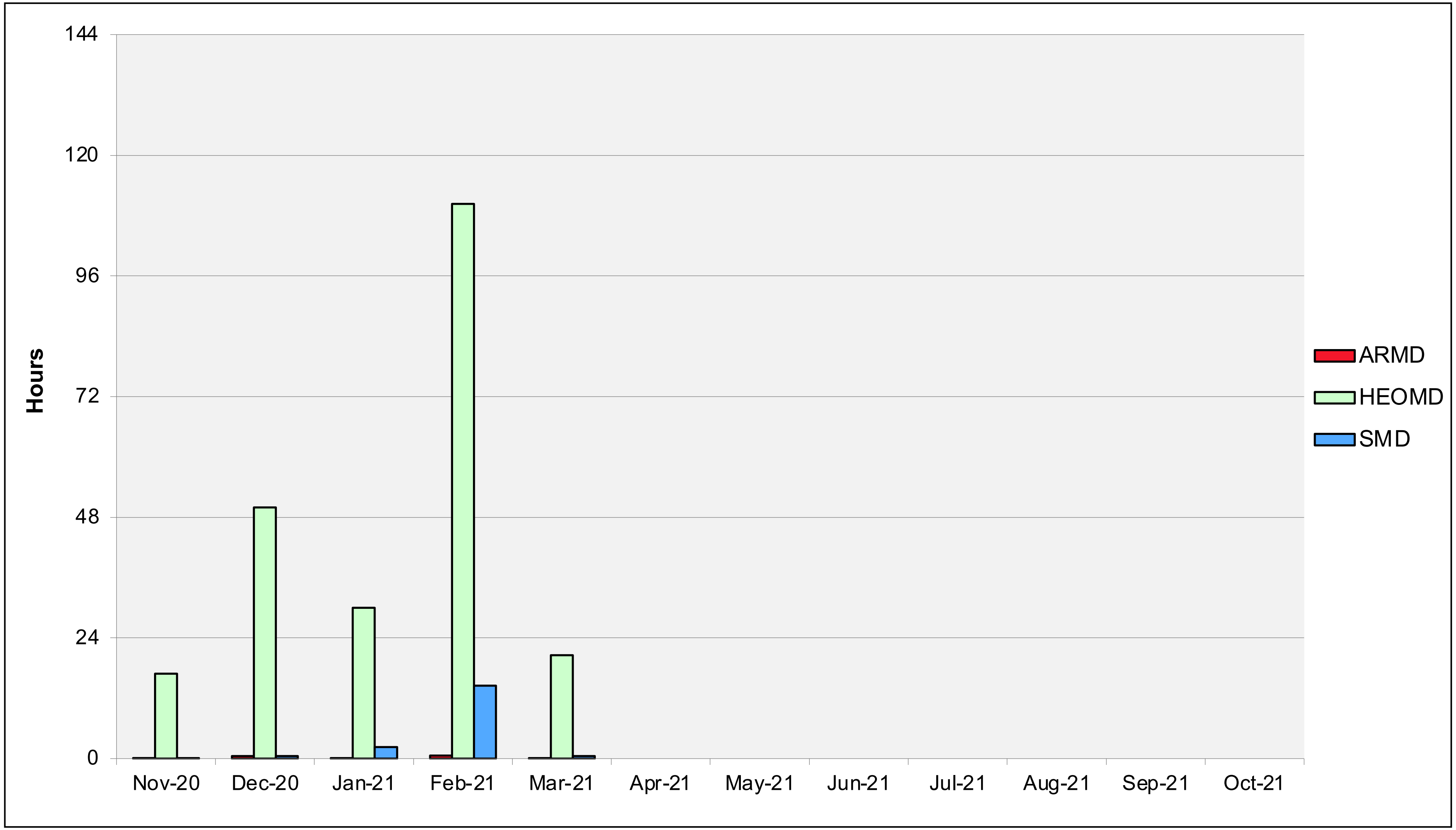
Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor